Supporting Information

Computation-Aided Development of Next-Generation Extractants for Trivalent Actinide and Lanthanide Separation

Xiaofan Yang[1#], Dong Fang[1,5#], Linjia Chen[3#], Yaoyang Liu[2], Shihui Wang[1], Lei Xu[4], Anyun Zhang[1], Jing Su[3*], Chao Xu[2*], Chengliang Xiao[1,5*]

1. College of Chemical and Biological Engineering, Zhejiang University, Hangzhou 310058, China

2. Institute of Nuclear and New Energy Technology, Tsinghua University, Beijing 100084, China

3. College of Chemistry, Sichuan University, Chengdu 610064, China

4. Institute of Nuclear-Agricultural Science, Key Laboratory of Nuclear Agricultural Sciences of Ministry of Agriculture and Zhejiang Province, Zhejiang University, Hangzhou 310058, China

5. Institute of Zhejiang University-Quzhou, Quzhou 324000, China

[#] These authors contributed equally to this work.

* Corresponding author: xiaoc@zju.edu.cn; xuchao@tsinghua.edu.cn; jingsu@scu.edu.cn

Content

S 1 Experimental Section

S 1.1 Chemicals and Reagents

The chemical reagents used in this work, such as 1-(trifluoromethyl)-3-nitrobenzene (F-3), and lanthanides nitrate, are all commercially obtained with analytical purity (AR), which were directly used without any further purification. Europium perchlorate was prepared by dissolving europium nitrate solid in excess perchloric acid (1 M $HClO_4$) and then heating and re-evaporating (120℃, 6 hours) solution three times. The operating temperature of solvent extraction, stripping, and titration experiments was controlled at 25 ± 1 ℃.

S 1.2 Synthesis of Extractants

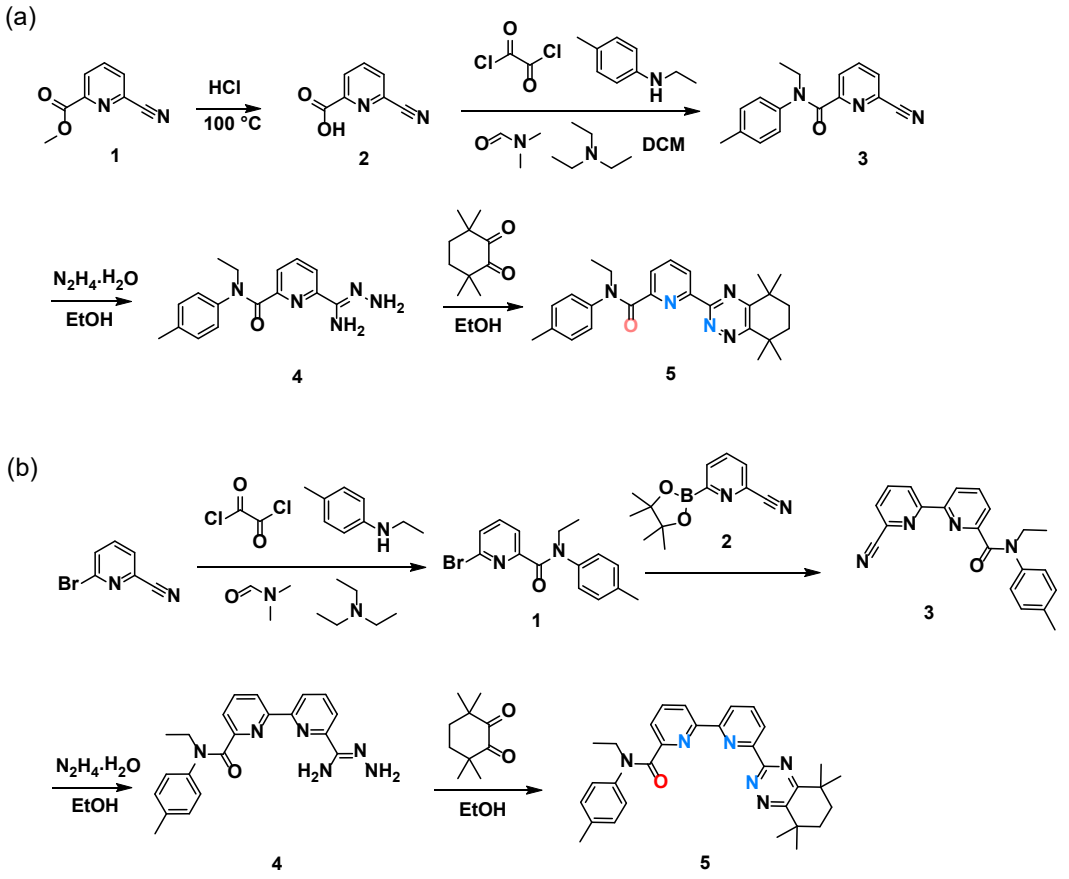


Figure S1. The synthesis route of (a) **L1** and (b) **L2**.

*S 1.2.1 Synthesis of **L1** extractant*

The synthesis method of **L1** extractant is shown in Figure S1(a): Compound **1** (6-cyano-2-pyridine carboxylic acid methyl ester, 1.0 g, 6.2 mmol) was weighed and added into 10 mL dilute hydrochloric acid solution with a concentration of 1 mol/L, and the reflux reaction was heated for 2 hours. After the reaction, it was cooled to room temperature, and a white solid was precipitated at the bottom of the container. Compound **2** (0.7 g) could be obtained by filtration.

Compound **2** (0.29 g, 2.0 mmol) was dissolved in 15 mL dichloromethane, followed by (0.25 g, 2.0 mmol) oxaloyl chloride and 2 drops of DMF solution, stirred until no gas was formed, and then N-ethyl-4-methylaniline (0.27 g, 2 mmol) was added for reaction for 12 hours. After the reaction was completed, a water quenching reaction was added, and 30 mL ethyl acetate was used for extraction 3 times. The organic phase was dried with Na_2SO_4, and the white solid **3** (0.39 g, 75% yield) was separated by column chromatography.

Compound **3** (0.52 g, 2.0 mmol) was weighed and dissolved in 20 mL ethanol solution, then 7 mL hydrazine hydrate was added and the reaction was complete after stirring for 4 hours. Then, a water quenching reaction was added, ethyl acetate extraction (15 mL × 3 times). The organic phase was collected from the separated liquid, and the yellow solid **4** (0.53 g, 89% yield) was separated by Na_2SO_4 drying and column chromatography.

Compound **4** (0.22 g, 0.66 mmol) and 3,3,6,6-tetramethylcyclohexane-1,2-dione (0.12 g, 0.72 mmol) were added to the solution of ethanol and triethylamine with v/v=10:1, heated to reflux, and the reaction was complete after 6 hours of agitation. Cooling to room temperature, quenching reaction with water, extraction with ethyl acetate (10 mL × 3 times). The organic phase was collected in a separate liquid, Na_2SO_4 was dried, and yellow solid **L1** (0.23 g, yield 82%) was separated by column chromatography.

*S1.2.2 Synthesis of **L2** extractant*

The synthesis method of **L2** extractant is shown in Figure S1(b). The compound 5-bromo-2-pyridinecarbonitrile (1.99 g, 10.9 mmol) was weighed and added to methylene chloride solution, followed by the addition of (1.38 g, 10.9 mmol) oxaloyl chloride and 4 drops of DMF solution, and stirred until no gas was formed. N-ethyl-4-methylaniline (1.05 g, 10.9 mmol) was added and the reaction lasted overnight (12 hours). Add water quenching reaction, and ethyl acetate extraction (30 mL × 3 times), the organic phase was collected by liquid separation, Na_2SO_4 drying, and white solid **1** (2.82 g, 81% yield) was separated by column chromatography.

Compound **1** (0.41 g, 1.2 mmol), compound **2** (0.26 g, 1.1 mmol), potassium carbonate (0.23 g, 1.6 mmol), tetrakis(triphenylphosphine)palladium (0.11 g, 0.11 mmol) were added to the glass reaction bottle, and vacuum filled with argon gas as protection gas. DMF and aqueous solution of v:v=10:1 was added to the reaction bottle, and the reaction was completed by heating and stirring under reflux overnight (12 hours). After cooling to room temperature, adding water quenching reaction, and ethyl acetate extraction (10 mL × 3 times), the organic phase was collected by liquid separation, Na_2SO_4 drying, and white solid **3** (0.13 g, 36% yield) was separated by column chromatography.

Compound **3** (0.34 g, 1.0 mmol) was dissolved in 15 mL ethanol solution, 4 mL hydrazine hydrate was added, and the reaction was complete after stirring for 5 hours. After the water quenching reaction, and ethyl acetate extraction (10 mL × 3 times), the organic phase was collected by liquid separation, Na_2SO_4 drying, and yellow solid **4** (0.34 g, 91% yield) was separated by column chromatography.

Compound **4** (0.34 g, 1.0 mmol) and 3,3,6,6-tetramethylcyclohexane-1,2-dione (0.18 g, 1.1 mmol) were added to the solution of ethanol and triethylamine with v:v=10:1, and the reaction was complete after heating and stirring under reflux for 5 hours. After cooling to room temperature, quenching reaction with water, and extraction with ethyl acetate (10 mL × 3 times), the organic phase was collected by liquid separation, Na_2SO_4 drying, yellow **L2** solid (0.44 g, 86% yield) was separated by column chromatography.

*S1.2.3 Synthesis of **L3** extractant*

Intermediate **1**: First, 7-methylquinoline (5 g, 35 mmol) was dissolved in dichloromethane (DCM), and 3-chloroperbenzoic acid (6.6 g, 38.5 mmol) was added, and the reaction was 7-12 hours at room temperature. With sodium bicarbonate solution quenching reaction, dichloromethane extraction, dried over Na_2SO_4, 7-methylquinoline oxide, directly used in the next reaction. 7-methylquinoline oxide (5 g, 31.4 mmol) was dissolved in anhydrous dichloromethane, and benzoyl chloride (6.6 g, 47.1 mmol) and trimethylsilyl cyanide (4.6 g, 47.1 mmol) were slowly added and reacted at room temperature for 7-12 hours. Sodium bicarbonate solution was added to quench reaction, dichloromethane was extracted, Na_2SO_4 was used to dry, and 2-cyano-7-methylquinoline was separated by column chromatography. 2-cyano-7-methylquinoline (5 g, 29.7 mmol) was dissolved in sulfuric acid solution (15 mL), and nitric acid (6.5 mL) was slowly added to the ice bath for 1 hour. Then the reaction liquid was introduced into the ice block for quenching reaction, dichloromethane extraction, Na_2SO_4 drying, and column chromatography to obtain 2-cyano-7-methyl-8-nitroquinoline. 2-cyano-7-methyl-8-nitroquinoline (5 g, 23.4 mmol) was dissolved in DMF (25 mL), followed by N,N-dimethylformamide dimethyl acetal (4.2 g, 35.1 mmol) for 7-12 hours. After stopping the reaction, the reaction liquid was poured into water, the solid was precipitated, and 2-cyano-7-(N, N-dimethylamine-vinyl)-8-nitro-quinoline solid was filtered, and the next step was direct reaction. 2-cyano-7-(N, N-dimethylamine-vinyl)-8-nitro-quinoline (2.7 g, 10.0 mmol) was dissolved in tetrahydrofuran and water (v:v = 1:1, 60 mL) solution, and sodium periodate (3.2 g, 15.0 mmol) was added for 6-8 hours. 2-cyano-7-aldehyde-8-nitro-quinoline was obtained by water quenching reaction, extraction by ethyl acetate, drying by Na_2SO_4, and separation by

column chromatography to afford the desired product. 2-cyano-7-aldehyde-8-nitro-quinoline (2.3 g, 10.0 mmol) was added into the solution of ethanol and acetic acid (v:v = 4:1, 40 mL), and iron powder (2.8 g, 50.0 mmol) was added, and heated to 50-80℃ for 4-8 hours. Then, it was filtered hot, dried with Na_2SO_4 by ethyl acetate extraction, and separated by column chromatography to obtain intermediate **1**.

Intermediate **2**: Add pyruvate (1.0 g, 11.4 mmol) to DCM (20 mL), then add oxaloyl chloride (1.4 g, 11.4 mmol) and 2 drops of DMF solution, stirring until no gas was produced. Then, N-ethyl-4-methylaniline (1.4 g, 11.4 mmol) was dissolved in dichloromethane (10 mL), slowly added to the reaction solution, and the reaction was carried out overnight at room temperature. The intermediate **2** was obtained by water quenching reaction, extraction by ethyl acetate, drying by Na_2SO_4, and separation by column chromatography to afford the desired product.

Intermediate **5**: Ethyl isobutyrate (6.27 g, 54 mmol) was added to 60 mL diethyl ether under Ar atmosphere at 0 ℃. Lithium diisopropylamide (55.34 mmol in THF solution) was added dropwise and then the mixture was stirred for 1 hour. Subsequently, ethylene di(ptoluenesulfonate) (10.0 g, 27.0 mmol) was added several times over 20 min and then the reaction mixture was refluxed under 45 ℃ over 24 hours. After the solid was filtered, the filtrate evaporated to obtain the crude product (5.2 g) which used without further purification. Sodium (3.1 g, 134 mmol) was added to 50 mL dry toluene under Ar atmosphere and then refluxed over 1 hour until the sodium melted. Subsequently, the diethyl 2,2,5,5-tetramethylhexanedioate (6.9 g, 26.9 mmol) and chlorotrimethylsilane (14.5 g, 134 mmol) were added, respectively. The reaction mixture was heated to 130 ℃ for 24 hours and then cooled to room temperature. The mixture was filtered through diatomaceous earth and then washed with diethyl ether, and the filtrate was concentrated under reduced pressure. The residue was purified by flash column chromatography to yield the 1,2-bis(trimethylsilyloxy)-3,3,6,6-tetramethylcyclohex-1-ene 12 (5.1 g, 16.2 mmol). Finally, all the previous product was dissolved in DCM and bromine (2.6 g, 16.2 mmol) was slowly added over 20 min. The reaction mixture was stirred at room temperature for 1 hour. Subsequently, the reaction was quenched with sodium thiosulfate (aq.) until the solution was pale yellow and was extracted with DCM (30 mL × 3). The combined organic layer was washed with brine (50 mL), dried over $MgSO_4$ and concentrated under reduced pressure. The residue was purified by flash column chromatography (DCM: PE = 5:3) to yield the intermediate **5** as yellow solid.

The synthesis method of **L3** extractant is shown in Figure 1(d). Intermediate **1** (0.4 g, 2 mmol) and intermediate **2** (0.4 g, 2.0 mmol) were added to 30 mL ethanol solution, then 0.2 mL ethanol

solution saturated with KOH was added and heated to 50 °C for 5 hours. Then the reaction was stopped and left at room temperature, without post-processing, directly used for the next reaction. The solution obtained in the previous step was directly added to 8 mL of 85% hydrazine hydrate solution and reacted overnight at room temperature. After the reaction, dilute with aqueous solution and extract with ethyl acetate (30 mL × 3 times). The organic phase was combined, dried with anhydrous sodium sulfate and separated by column chromatography (DCM: MeOH = 5:1) to obtain yellow solid **4**. Compound **4** (0.4 g, 1.0 mmol) and 3,3,6,6-tetramethylcyclohexane-1,2-dione (compound **5**) were heated in a mixture of 20 mL of tetrahydrofuran and triethylamine (v/v = 10:1) for 8 hours of reflux reaction, then the heating was stopped and cooled to room temperature. Then dilute with water, extract with ethyl acetate (20 mL) 3 times, and dry with Na_2SO_4. The product was obtained by column chromatography (DCM: MeOH = 10:1) and a yellowish solid (**L3**) was obtained.

S 1.3 Solvent Extraction and Stripping

The distribution ratio (*D*), the extraction efficiency (*E*, %) and the stripping efficiency (*S*, %) were calculated as follows:

$$D = \frac{C_{org.}}{C_{aq.}} \tag{S1}$$

$$E(\%) = \frac{C_{org.}}{C_{F.}} \times \frac{V_{org.}}{V_{F.}} \times 100\% \tag{S2}$$

$$S(\%) = \frac{C_{str.aq.}}{C_{ext.org.}} \times 100\% \tag{S3}$$

The general extraction equilibriums can be described by equation (S4). (The subscript (org.) or (aq.) indicate that the substance exists in the organic phase or aqueous phase)

$$M^{m+}_{(aq.)} + mNO^{-}_{3(aq.)} + nL_{(org.)} \rightleftharpoons \mathrm{M}(NO_3)_m(L)_{n_{(org.)}} \tag{S4}$$

n is the coordination number of ligand to metal ion, the corresponding extraction equilibrium constant, K_{ex}, can be defined as:

$$K_{ex} = \frac{[\mathrm{M}(NO_3)_m(L)_n]_{(org.)}}{[M^{m+}]_{(aq.)}[NO_3^-]^m_{(aq.)}[L]^n_{(org.)}} \tag{S5}$$

The distribution ratio of metal ion, D_M, can be represented as:

$$D_M = \frac{[\mathrm{M}(NO_3)_m(L)_n]_{(org.)}}{[M^{m+}]_{(aq.)}} \tag{S6}$$

By substituting equation (S6) into equation (S5), and transforming Eq. (S6) into the log

form, equation (S7), (S8), and (S9) are obtained:

$$\mathrm{Log}D_M = logK_{ex} + nlog[L]_{(org.)} + mlog[NO_3]_{(aq.)} \quad (S7)$$

$$\mathrm{Log}D_M = nlog[L]_{(org.)} + C_1 \quad (C_1 = logK_{ex} + mlog[NO_3]_{(aq.)}) \quad (S8)$$

$$\mathrm{Log}D_M = mlog[NO_3]_{(aq.)} + C_2 \quad (C_2 = logK_{ex} + nlog[L]_{(org.)}) \quad (S9)$$

C_1 and C_2 are the constants when the corresponding condition is controlled. Based on above analysis, keeping the concentration of nitric acid constant, the slope of log-log plot regarding D vs. initial [L] present the number of extractant molecules coordinated to metal ion in the organic phase.

S 2 Results and Discussion

S 2.1 Theoretical Prediction and Screening

S 2.1.1 The Most Stable Conformation of ML-type Complexes using DFT Calculations

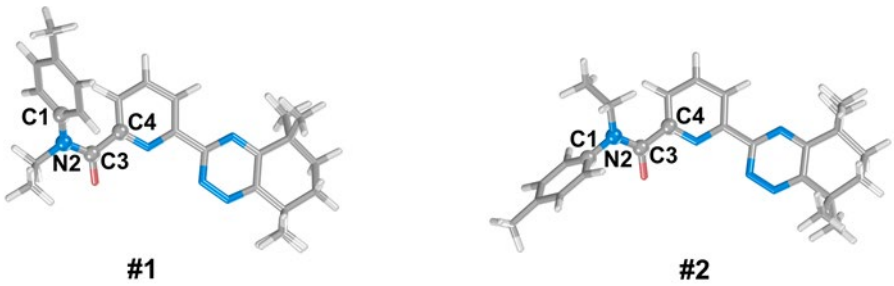


Figure S2. Comparison of two configurations of the ligand in the ML-type complexes. For configuration #1, the benzyl group and the central skeleton are on the same side of the N2-C3 bond, and the absolute value of the dihedral angle C1-N2-C3-C4 is less than 90 degrees. For configuration #2, the benzyl group and the central skeleton are on opposite sides of the N2-C3 bond, and the absolute value of the dihedral angle C1-N2-C3-C4 is greater than 90 degrees.

Table S1. Relative energies (ΔE in kcal/mol) of two isomers of Am(**L**)$(NO_3)_3$ (**L**=**L1**, **L2**, **L3**) complexes.

Isomers	Am(**L1**)$(NO_3)_3$	Am(**L2**)$(NO_3)_3$	Am(**L3**)$(NO_3)_3$
is1	0	0	0
is2	2.27	2.37	3.10

Table S2. Relative energies (ΔE in kcal/mol) of two isomers of Eu(**L**)$(NO_3)_3$ (**L**=**L1**, **L2**, **L3**) complexes.

Isomers	Eu(**L1**)$(NO_3)_3$	Eu(**L2**)$(NO_3)_3$	Eu(**L3**)$(NO_3)_3$
is1	0	0	0
is2	3.07	2.61	2.74

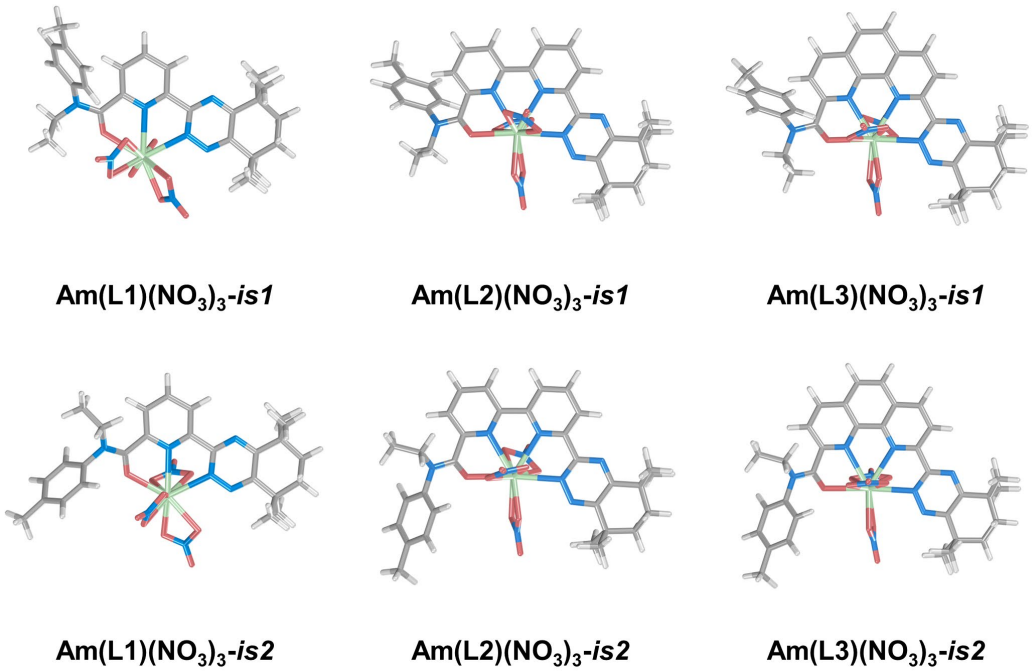


Figure S3. Optimized structures of two isomers of Am(**L**)$(NO_3)_3$ (**L**=**L1**, **L2**, **L3**) complexes labelled by Am(**L**)$(NO_3)_3$-*is1* and Am(**L**)$(NO_3)_3$-*is2*, respectively, with the ligand adopting configuration #1 and #2, respectively, shown in Figure S2.

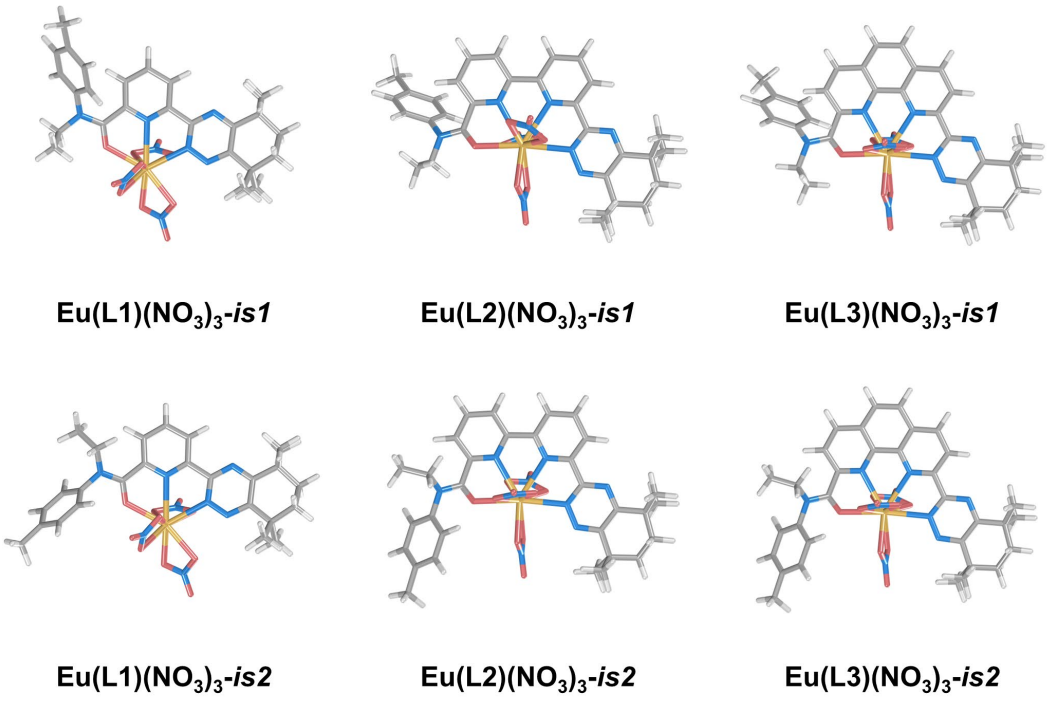


Figure S4. Optimized structures of two isomers of Eu(**L**)$(NO_3)_3$ (**L**=**L1**, **L2**, **L3**) complexes labelled by Eu(**L**)$(NO_3)_3$-*is1* and Eu(**L**)$(NO_3)_3$-*is2*, respectively, with the ligand adopting configuration #1 and #2, respectively, shown in Figure S2.

S 2.1.2 Bonding Analysis of ML-Type Complexes

Table S3. Calculated M-O and M-N Bond Lengths (Å) of the M(**L**)$(NO_3)_3$ (M=Am(III), Eu(III))[a]

Complexes	M-O		M-N_1		M-N_2		M-N_3	
	Am	Eu	Am	Eu	Am	Eu	Am	Eu
M(**L1**)$(NO_3)_3$	2.526	2.444	2.630	2.628	-	-	2.599	2.620
M(**L2**)$(NO_3)_3$	2.499	2.461	2.647	2.614	2.683	2.651	2.584	2.569
M(**L3**)$(NO_3)_3$	2.512	2.465	2.637	2.606	2.674	2.639	2.607	2.573

[a]O: The O atom in the amide side chain. N_1, N_2: The N atom in the central skeleton. N_3: The N atom in the triazine side chain.

Table S4. Bond order analysis of [M(**L**)$(NO_3)_3$] (M=Am(III), Eu(III)) complexes.[a]

Complexes	Bond Orders	M-O		M-N_1		M-N_2		M-N_3	
		Am	Eu	Am	Eu	Am	Eu	Am	Eu
M(**L1**)$(NO_3)_3$	MAYER	0.258	0.233	0.196	0.131	-	-	0.224	0.149
	N-M	1.139	1.097	0.670	0.652	-	-	0.516	0.456
M(**L2**)$(NO_3)_3$	MAYER	0.259	0.228	0.180	0.145	0.176	0.145	0.185	0.143
	N-M	1.110	1.078	0.665	0.634	0.672	0.638	0.464	0.433
M(**L3**)$(NO_3)_3$	MAYER	0.256	0.224	0.176	0.140	0.180	0.143	0.182	0.140
	N-M	1.111	1.069	0.655	0.629	0.670	0.635	0.458	0.424

[a]Bond-orders calculated from two-electron valence indices based on partitioning of tr(ΔP^2) (4-index set).

Table S5. Energy decomposition analysis of the total bonding interaction (in kcal/mol) between fragments $M(NO_3)_3$ and ligand in M(**L**)$(NO_3)_3$ (M=Am(III), Eu(III)) complexes.

Complexes	Metal	Steric interaction			orbital interaction	Total bonding energy[b]	orb%[c]
		electrostatic	Pauli	Sum[a]			
M(**L1**)$(NO_3)_3$	Am(III)	-108.60	105.75	-2.85	-62.38	-65.23	36.48%
	Eu(III)	-91.86	84.83	-7.03	-51.68	-58.70	36.00%
M(**L2**)$(NO_3)_3$	Am(III)	-140.76	140.32	-0.44	-79.68	-80.12	36.15%
	Eu(III)	-127.65	125.04	-2.61	-70.70	-73.30	35.64%
M(**L3**)$(NO_3)_3$	Am(III)	-138.23	136.86	-1.37	-79.32	-80.69	36.46%
	Eu(III)	-126.26	122.67	-3.57	-70.70	-74.30	35.90%

[a]Steric interaction is the sum of electrostatic interactions and Pauli interactions.

[b]Total bonding energy is the sum of steric interactions and orbital interactions.

[c]The percentage of orbital interactions in the total sum of electrostatic and orbital interactions.

S 2.1.3 ETS-NOCV:

The natural orbitals for chemical valence (NOCV) deformation densities of alpha and beta spin, along with their associated energy contributions (ΔE_k in kcal/mol), corresponding eigenvalues, and the symmetrized fragment orbitals (SFO), are provided. The contour values are 0.0003 a.u. for the NOCV orbitals and 0.03 a.u. for the SFO, respectively. Blue represents positive, and red represents negative. The value v quantifies the number of electrons transferred

between the SFO, in which negative and positive values respectively represent electron loss and electron gain. The compositions of the acceptor orbitals are also provided.

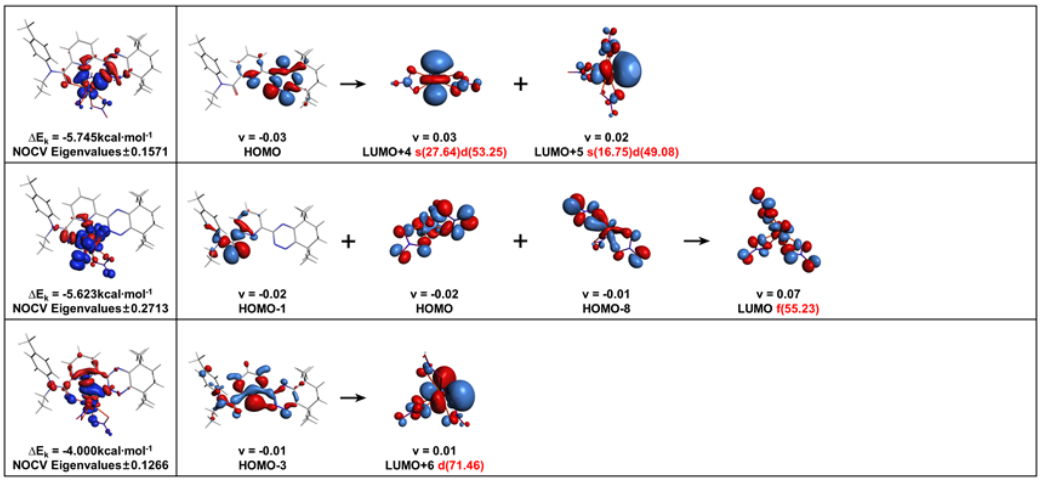


Figure S5. The ETS-NOCV analysis of the alpha spin in Eu(**L1**)$(NO_3)_3$ complex.

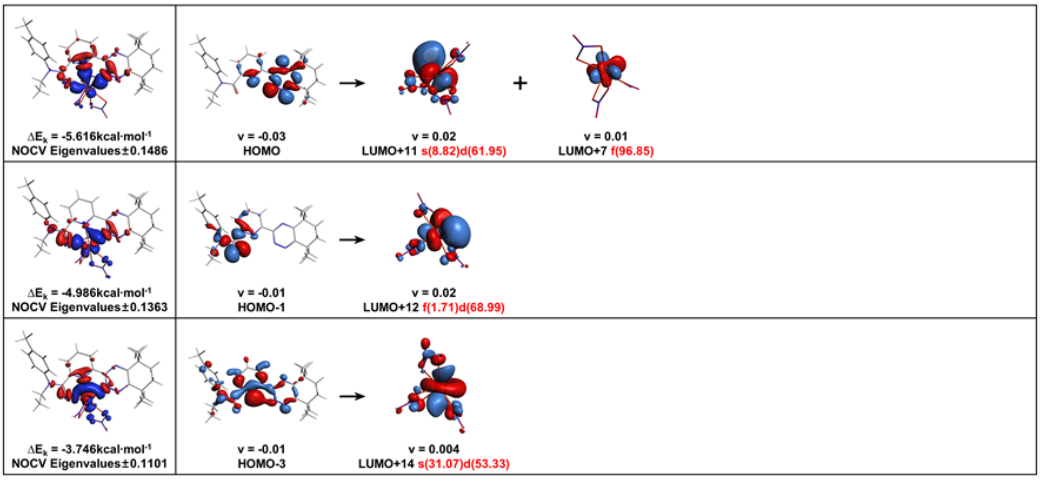


Figure S6. The ETS-NOCV analysis of the beta spin in Eu(**L1**)$(NO_3)_3$ complex.

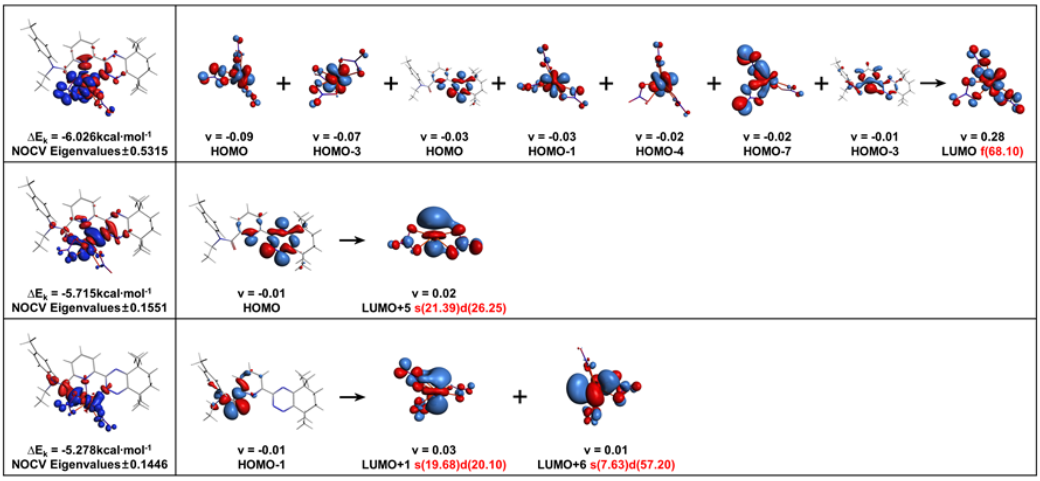


Figure S7. The ETS-NOCV analysis of the alpha spin in Am(**L1**)$(NO_3)_3$ complex.

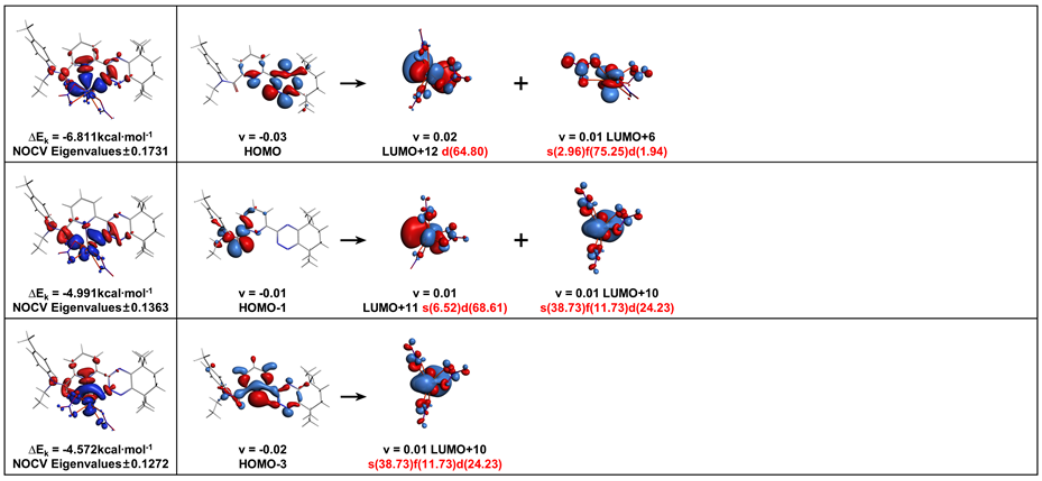


Figure S8. The ETS-NOCV analysis of the beta spin in Am(**L1**)$(NO_3)_3$ complex.

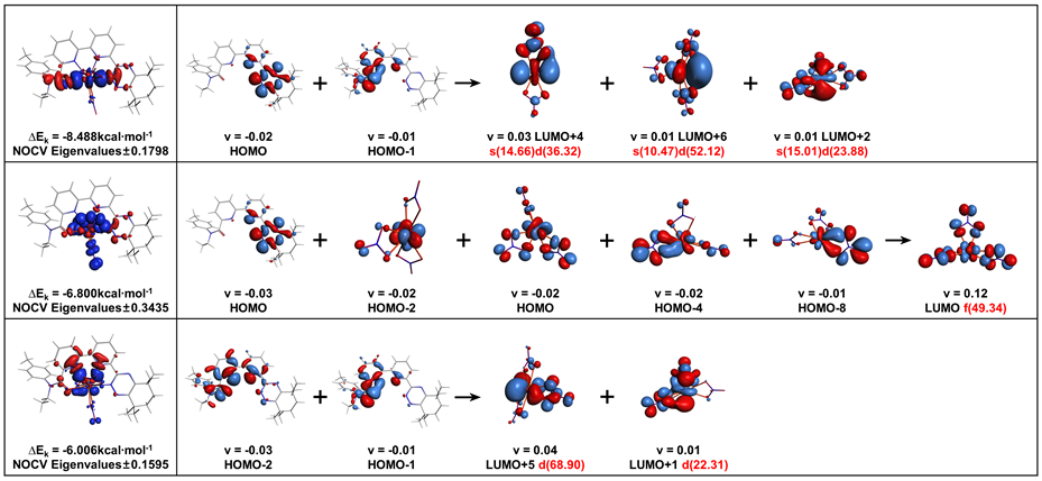


Figure S9. The ETS-NOCV analysis of the alpha spin in Eu(**L2**)$(NO_3)_3$ complex.

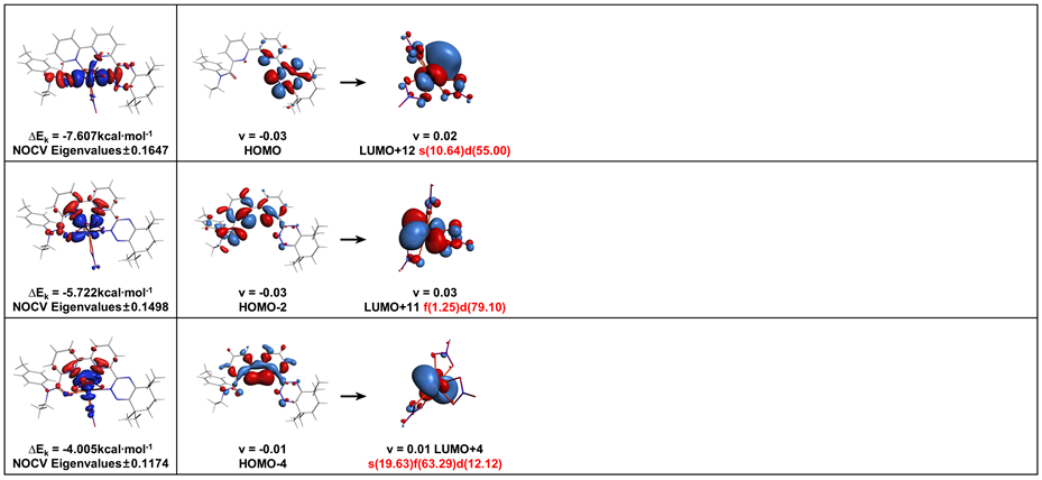


Figure S10. The ETS-NOCV analysis of the beta spin in Eu(**L2**)$(NO_3)_3$ complex.

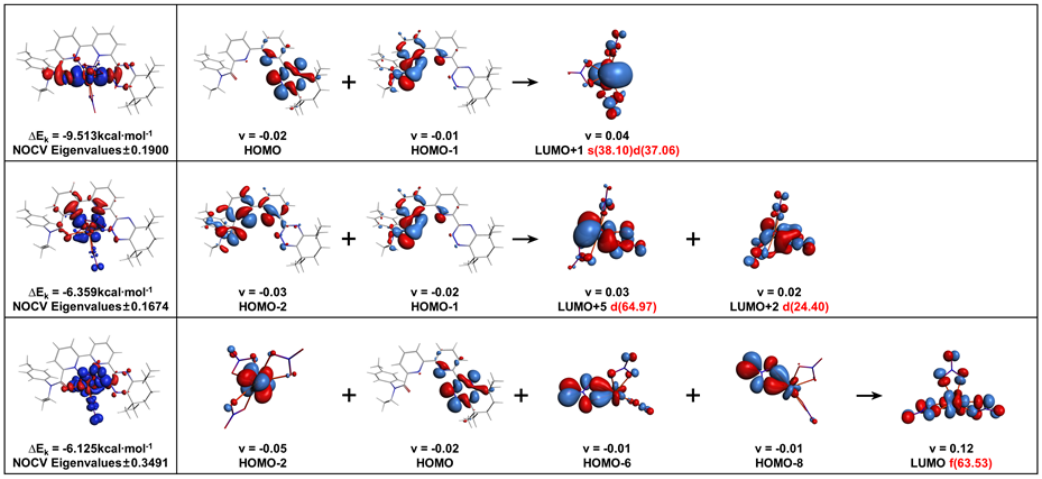


Figure S11. The ETS-NOCV analysis of the alpha spin in Am(**L2**)$(NO_3)_3$ complex.

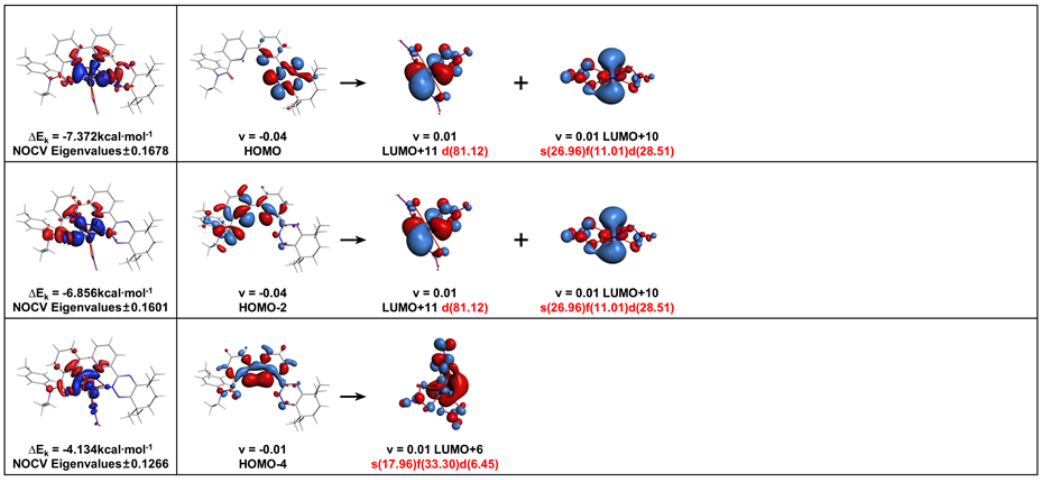


Figure S12. The ETS-NOCV analysis of the beta spin in Am(**L2**)$(NO_3)_3$ complex.

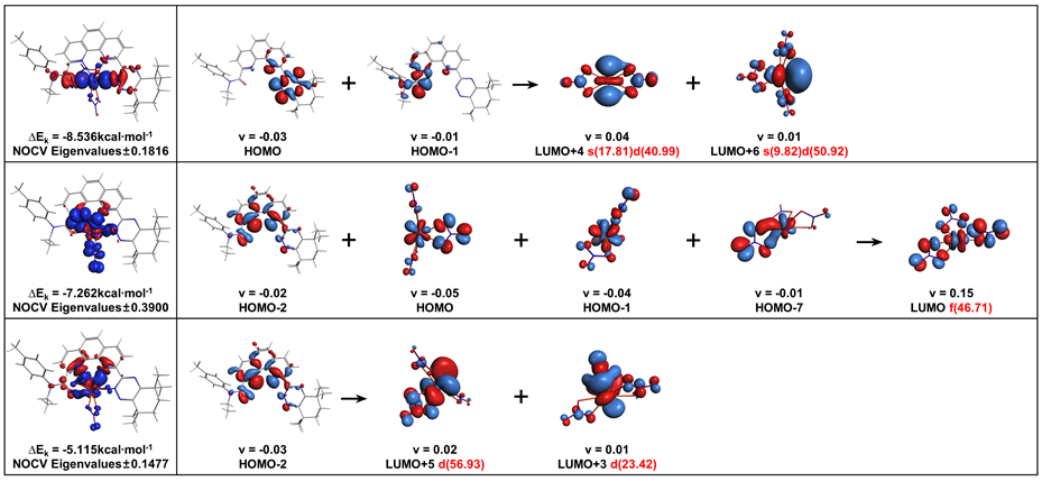


Figure S13. The ETS-NOCV analysis of the alpha spin in Eu(**L3**)$(NO_3)_3$ complex.

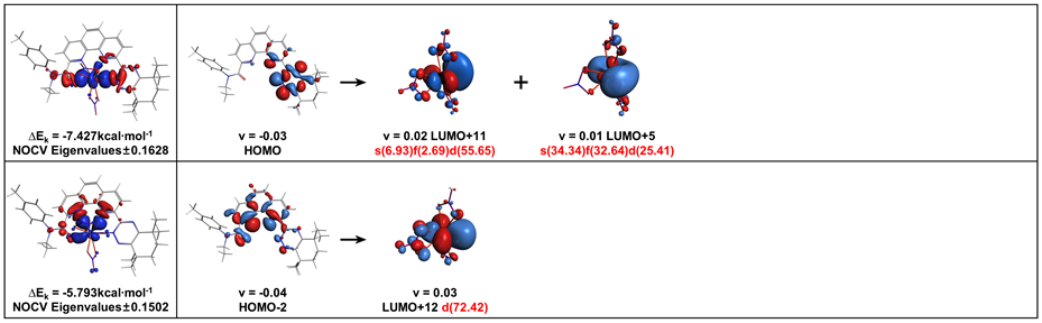


Figure S14. The ETS-NOCV analysis of the beta spin in Eu(**L3**)$(NO_3)_3$ complex.

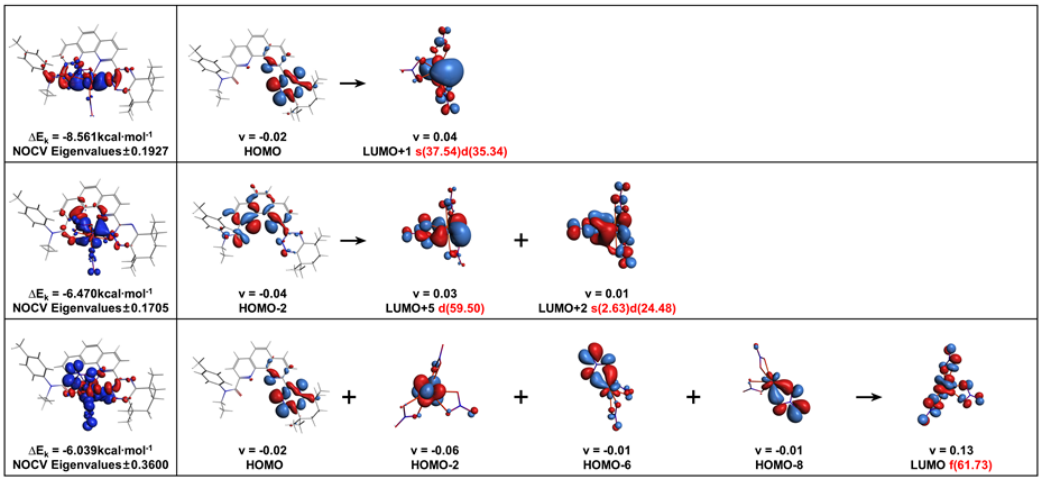


Figure S15. The ETS-NOCV analysis of the alpha spin in Am(**L3**)$(NO_3)_3$ complex.

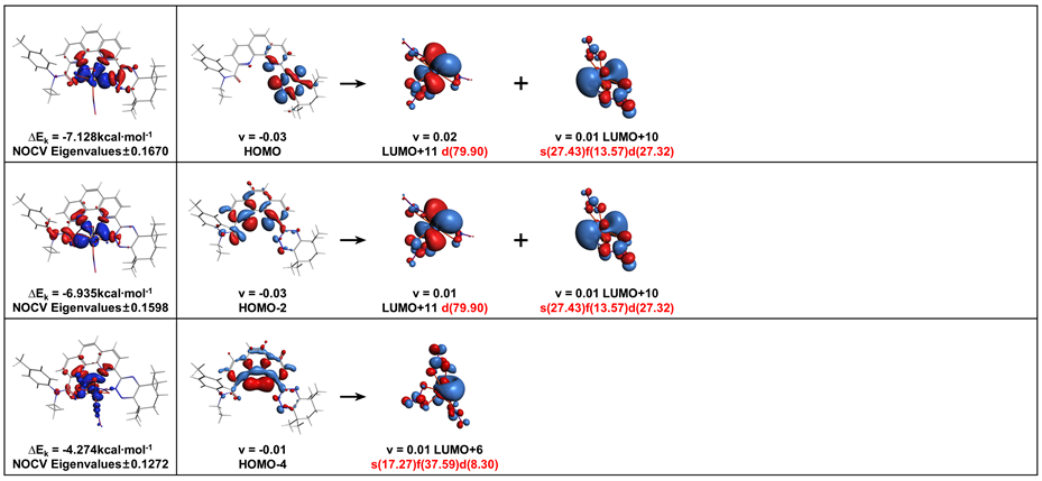


Figure S16. The ETS-NOCV analysis of the beta spin in Am(**L3**)$(NO_3)_3$ complex.

S 2.1.4 Thermodynamic calculations and orbital analysis of ML-type Complexes

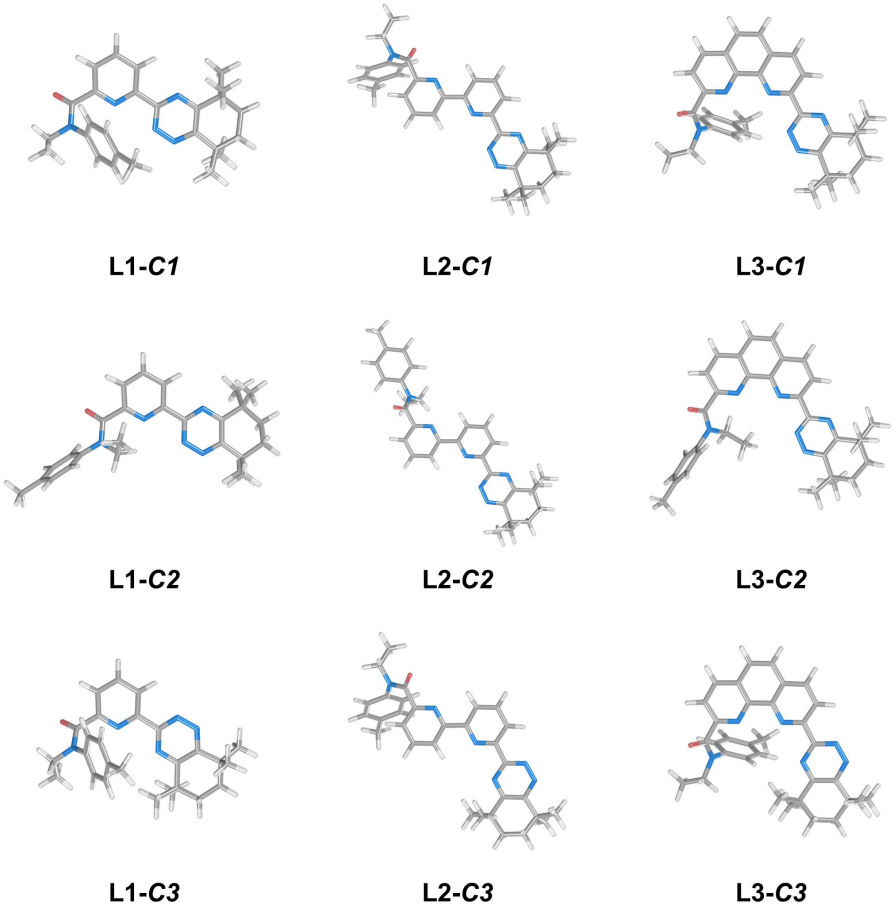


Figure S17. Optimized structures of **L1**, **L2** and **L3** in gas phase. C1: The most stable conformation and are employed for thermodynamic calculations. C2: Obtained by rotating the amide side chain during the initial modeling process based on C1. In this case, the orientation of the O atom in the optimized conformation remains unchanged regardless of rotation. C3: Obtained by rotating the triazine side chain during the initial modeling process based on C1.

Table S6. Relative Energies (ΔE in kcal/mol) of Various Conformations in the Ligand.

Conformations	**L1**	**L2**	**L3**
C1	0	0	0
C2	3.65	1.64	0.77
C3	0.26	1.98	0.30

The initial structures for the free ligands were constructed by modifying similar structures found in published literature. During the modeling of these initial structures, we considered the conformational changes caused by the rotation of single bonds in the ligands. The three conformations of each ligand are from the convergence results of multiple initial conformations.

Table S7. Calculated Gibbs free energies (ΔG in kcal/mol) of the complexation reactions of ligands with $[M(NO_3)(H_2O)_8]^{2+}$ and the difference in ΔG between Am and Eu ($\Delta\Delta G$ in kcal/mol) in nitrobenzene.[a]

Extraction reaction	ΔG_{ext}		$\Delta\Delta G_{ext(Am-Eu)}$
	Am	Eu	
$[M(NO_3)(H_2O)_8]^{2+}$ + **L1** + $2NO_3^-$ = M(**L1**)$(NO_3)_3$ + $8H_2O$	-74.84	-74.07	-0.77
$[M(NO_3)(H_2O)_8]^{2+}$ + **L2** + $2NO_3^-$ = M(**L2**)$(NO_3)_3$ + $8H_2O$	-80.02	-76.90	-3.12
$[M(NO_3)(H_2O)_8]^{2+}$ + **L3** + $2NO_3^-$ = M(**L3**)$(NO_3)_3$ + $8H_2O$	-83.48	-79.74	-3.63

[a]Due to the absence of parameters for 1-(trifluoromethyl)-3-nitrobenzene solvent in the solvation model, nitrobenzene, which has a similar structure, was used as a substitute. As our focus is on the relative values of $\Delta\Delta G$, the impact of the solvation on which is not significant, this substitution is reasonable.

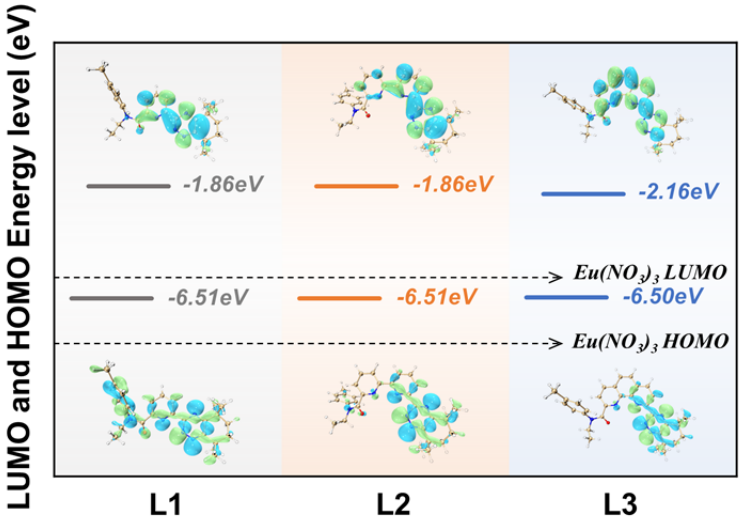


Figure S18. Frontier molecular orbital energy level diagram of **L1**, **L2**, and **L3** fragments in Eu(**L**)$(NO_3)_3$. The envelopes of HOMO and LUMO are given with contour values of 0.02 a.u.

S 2.2 Organic Synthesis

*S 2.2.1 Intermediate **1***

^{1}H NMR (500 MHz, $CDCl_3$) δ 10.01 (s, 1H), 8.15 (d, J = 8.5 Hz, 1H), 7.78 (d, J = 8.5 Hz, 1H), 7.68 (d, J = 8.5 Hz, 1H), 7.05 (d, J = 8.5 Hz, 1H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 192.88, 148.66, 138.88, 137.10, 133.71, 132.13, 130.37, 126.50, 117.32, 114.02, 112.67.

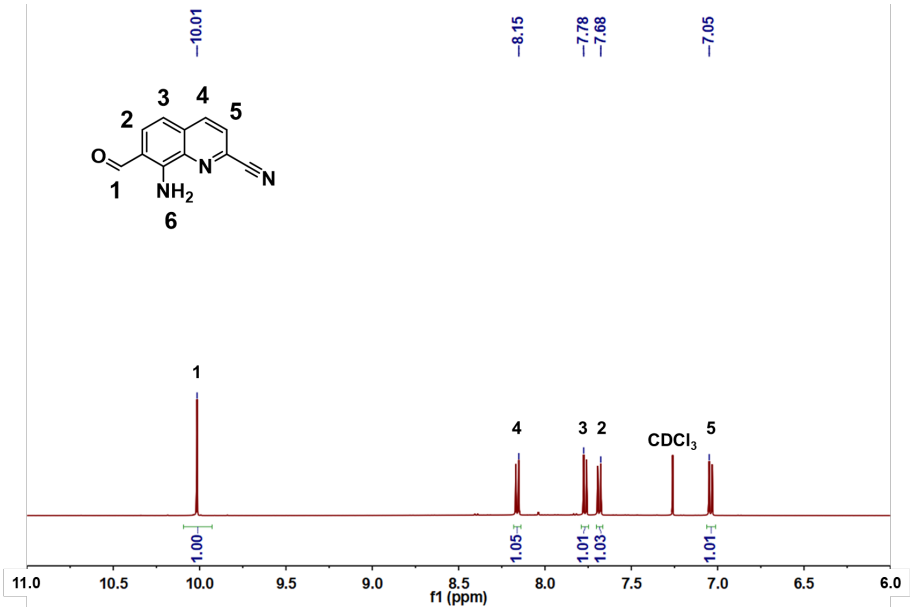


Figure S19. The ^{1}H NMR spectrum of 8-amino-7-formylquinoline-2-nitrile.

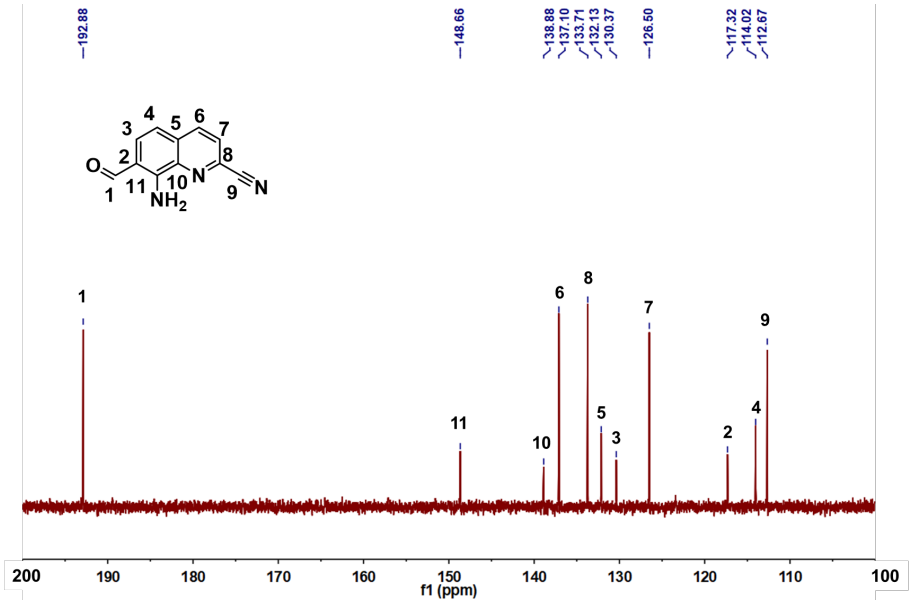


Figure S20. The ^{13}C NMR spectrum of 8-amino-7-formylquinoline-2-nitrile.

*S 2.2.2 Intermediate **2***

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.17 (d, J = 8.0 Hz, 2H), 7.04 (d, J = 8.0 Hz, 2H), 3.79 (q, J = 7.0 Hz, 2H), 2.35 (s, 3H), 2.17 (s, 3H), 1.16 (t, J = 7.0 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 198.32, 166.96, 138.53, 136.98, 130.29, 127.58, 43.60, 27.77, 21.10, 12.63.

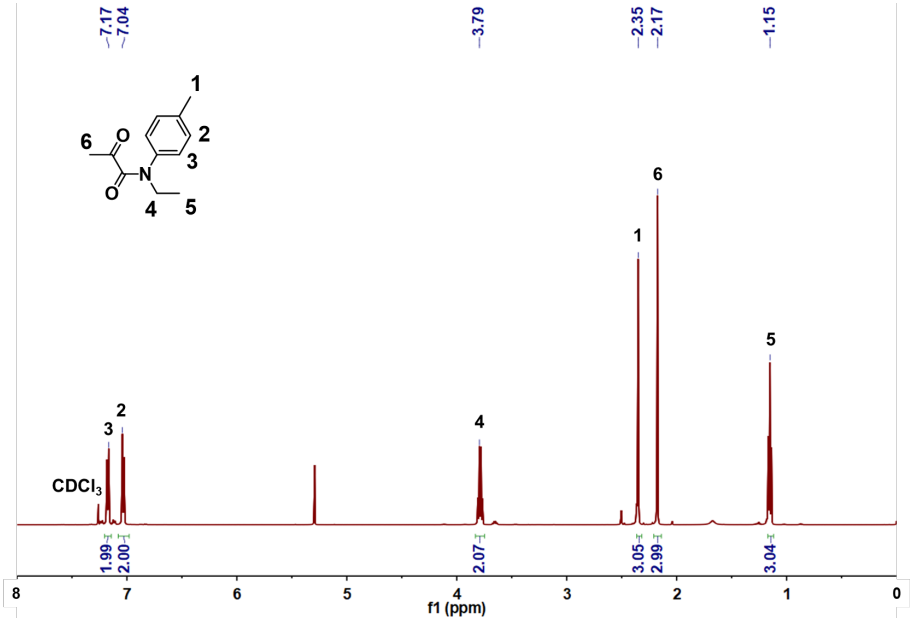


Figure S21. The ^{1}H NMR spectrum of N-ethyl-2-oxo-N-(p-tolyl)propanamide.

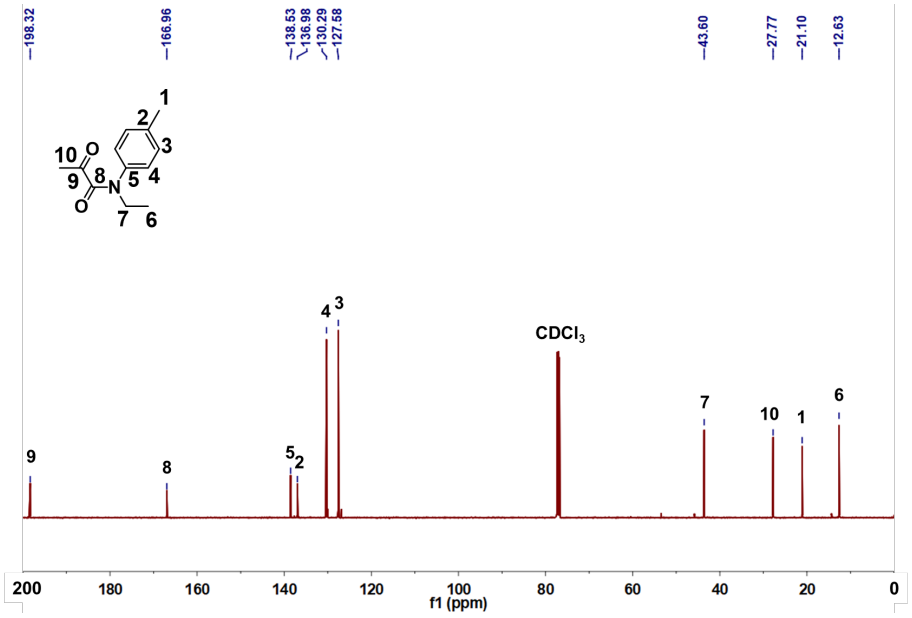


Figure S22. The ^{13}C NMR spectrum of N-ethyl-2-oxo-N-(p-tolyl)propanamide.

S 2.2.3 Intermediate ***5***

^{1}H NMR (500 MHz, $CDCl_3$) δ 1.86 (s, 4H), 1.15 (s, 12H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 207.40, 48.68, 34.67, 22.96.

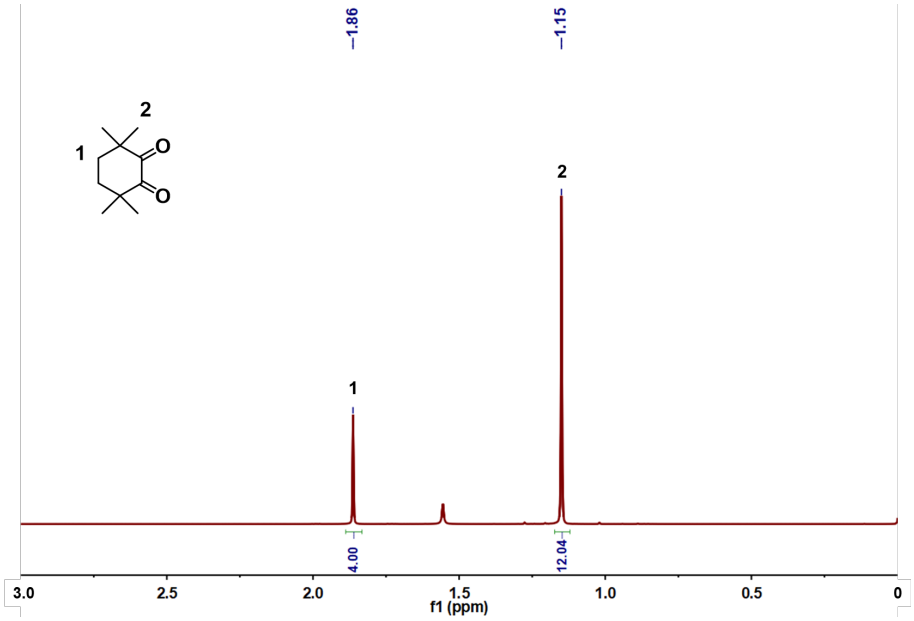


Figure S23. The ^{1}H NMR spectrum of 3,3,6,6-tetramethylcyclohexane-1,2-dione.

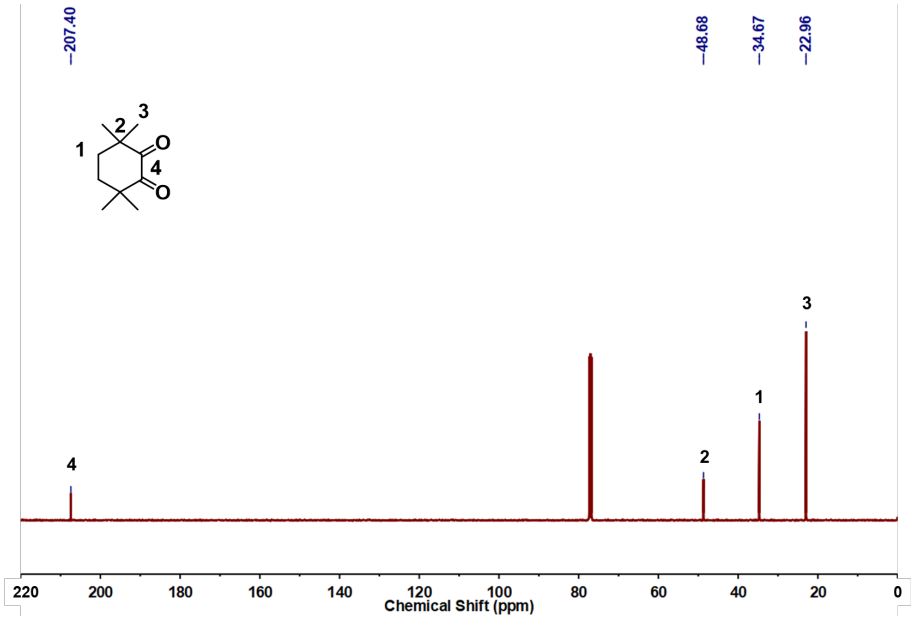


Figure S24. The ^{13}C NMR spectrum of 3,3,6,6-tetramethylcyclohexane-1,2-dione.

S 2.2.4 ***L1*** *extractant*

^{1}H NMR (500 MHz, Methanol-d4) δ8.33 (d, J = 8.0 Hz, 1H), 7.88 (t, J = 8.0 Hz, 1H), 7.51 (d, J = 8.0 Hz, 2H), 7.11 (d, J = 8.5 Hz, 2H), 7.00 (d, J = 8.0 Hz, 2H), 4.02 (q, J = 7.0 Hz, 2H), 2.16 (s, 3H), 1.91 (s, 4H), 1.50 (s, 6H), 1.44 (s, 6H), 1.26 (t, J = 7.0 Hz, 3H). **ESI-HRMS**: $[C_{26}H_{31}N_5O+H]^+$ Theoretical value: m/z = 430.2601, Actual value: m/z = 430.2607; $[C_{26}H_{31}N_5O+Na]^+$ Theoretical value: m/z = 452.2421, Actual value: m/z = 452.2462; [2 $C_{26}H_{31}N_5O+Na]^+$ Theoretical value: m/z = 881.4949, Actual value: m/z = 881.4958. **Organic element analysis:** $C_{26}H_{31}N_5O$ Theoretical value: C = 72.70%, H = 7.27%, N = 16.30%; Actual value: C = 72.56%, H = 7.30%, N = 16.44%.

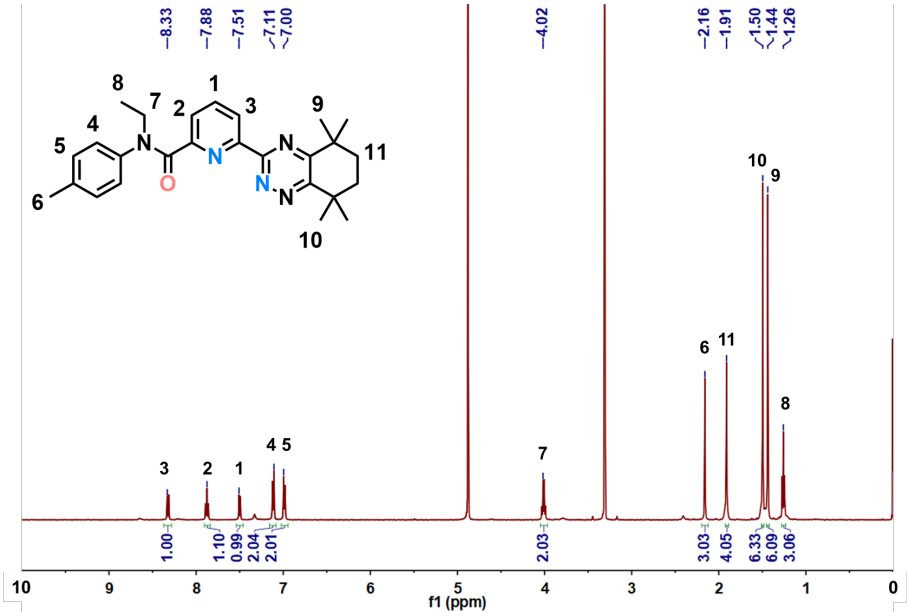


Figure S25. The ^{1}H NMR spectrum of **L1** extractant.

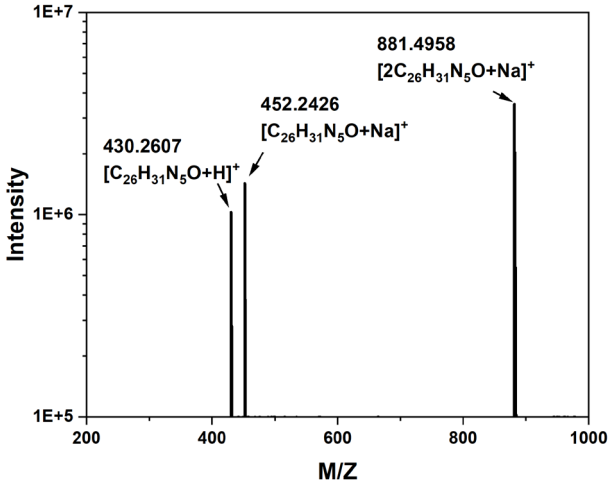


Figure S26. The ESI-MS result of **L1** extractant.

S 2.2.5 ***L2*** *extractant*

^{1}H NMR (500 MHz, Methanol-d4) δ8.62 (d, J = 8.0 Hz, 1H), 8,46 (d, J = 7,5 Hz, 1H), 8.06 (m, 2H), 7.90 (t, J = 8.0 Hz, 1H), 7.64 (d, J = 7.5 Hz, 1H),7.08 (s, 4H), 4.05 (q, J = 7.0 Hz, 2 h), 2.20 (s, 3H), 1.93 (s, 4H), 1.51 (s, 6H), 1.47 (s, 6H), 1.27 (t, J = 7.0 Hz, 3H). **ESI-HRMS**: $[C_{33}H_{34}N_6O+H]^+$ Theoretical value: m/z =507.2867, Actual value: m/z = 507.2867; $[C_{33}H_{34}N_6O+Na]^+$ Theoretical value: m/z = 529.2686, Actual value: m/z = 529.2683; [2 $C_{33}H_{34}N_6O+Na]^+$ Theoretical value: m/z = 1035.5480, Actual value: m/z = 1035.5464. **Organic element analysis:** $C_{33}H_{34}N_6O$ Theoretical value: C = 73.49%, H = 6.76%, N = 16.59%; Actual value: C = 73.44%, H = 6.74%, N = 16.72%.

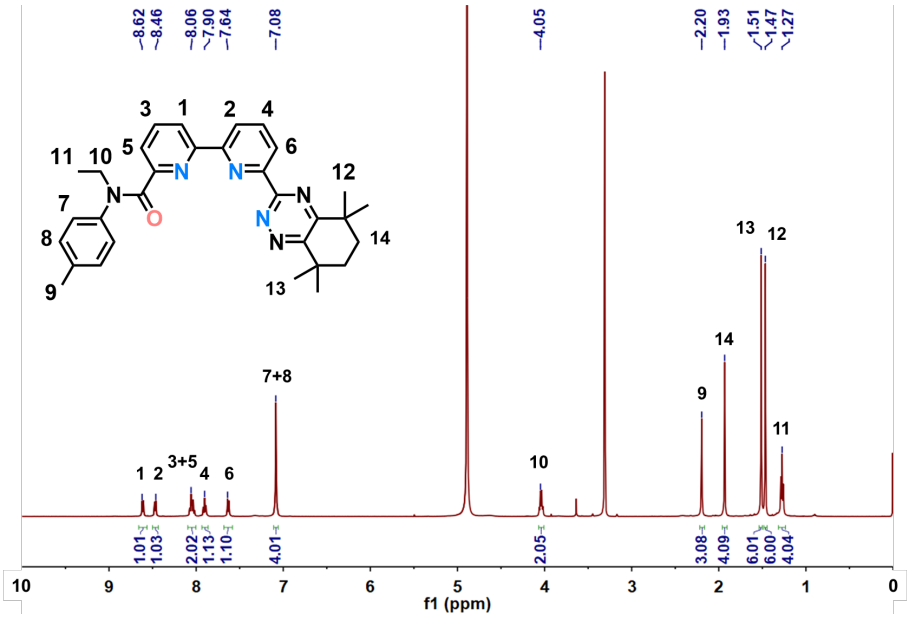


Figure S27. The ^{1}H NMR spectrum of **L2** extractant.

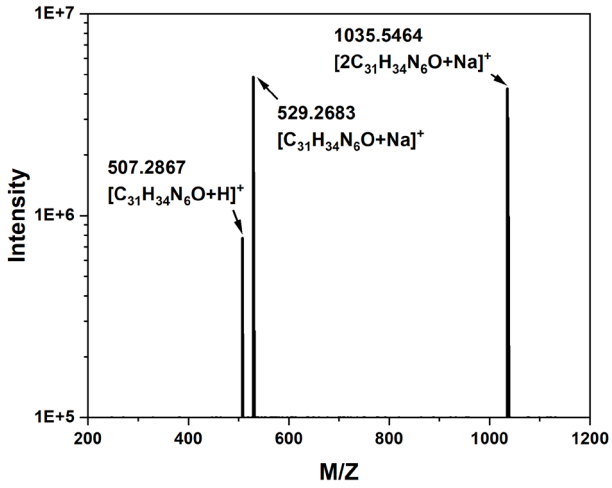


Figure S28. The ESI-MS result of **L2** extractant.

S 2.2.6 ***L3*** *extractant*

^{1}H NMR (500 MHz, Methanol-d4) δ8.82 (d, J = 8.5Hz, 1H), 8.71 (d, J = 8.0Hz, 1H), 8.23 (d, J = 7.5Hz, 1H), 8.10 (d, J = 8.5 Hz, 1H), 8.00 (d, J = 8.5 Hz, 1H), 7.39 (d, J = 7.5 Hz, 1H), 7.14 (d, J = 8.0 Hz, 2H), 6.94 (d, J = 7.0 Hz, 2H), 3.81 (q, J = 7.0 Hz, 2H), 2.19 (s, 3H), 1.79 (d, J = 25 Hz, 4H), 1.40 (s, 6H), 0.90 (s, 9H). **ESI-HRMS**: $[C_{33}H_{34}N_6O+H]^+$ Theoretical value: m/z = 531.2867; Actual value: 531.2871; $[C_{33}H_{34}N_6O+Na]^+$ Theoretical value: m/z = 553.2686; Actual value: 553.2688; $[2C_{33}H_{34}N_6O+Na]^+$ Theoretical value: m/z = 1083.5480; Actual value: 1083.5482. **Organic element analysis:** $C_{31}H_{34}N_6O$ Theoretical value: C = 73.49%, H = 6.76%, N = 16.59%; Actual value: C = 74.64%, H = 6.15%, N = 15.82%.

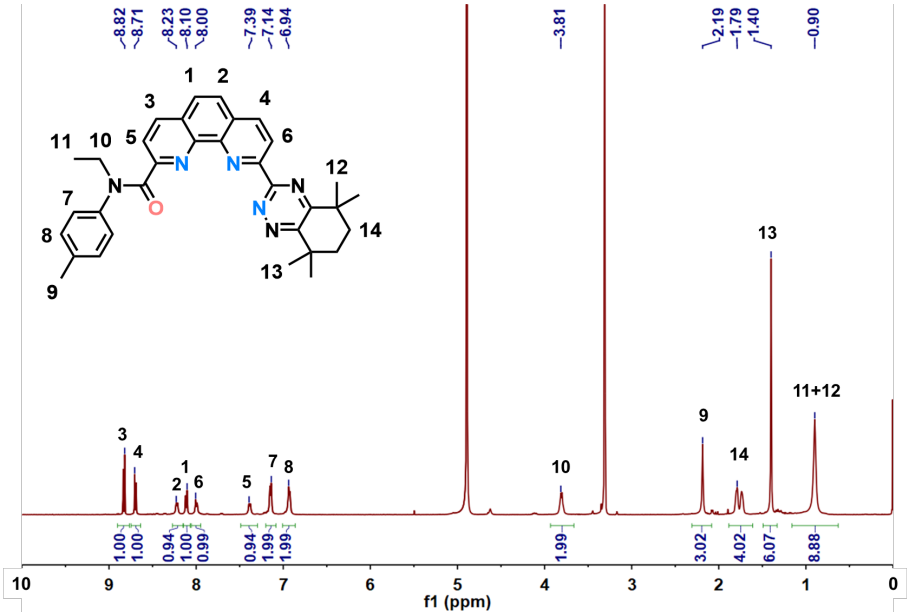


Figure S29. The ^{1}H NMR spectrum of **L3** extractant.

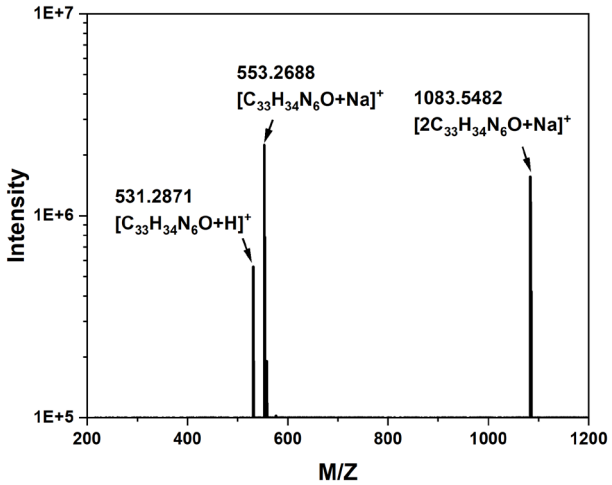


Figure S30. ESI-MS spectrum of **L3** extractant.

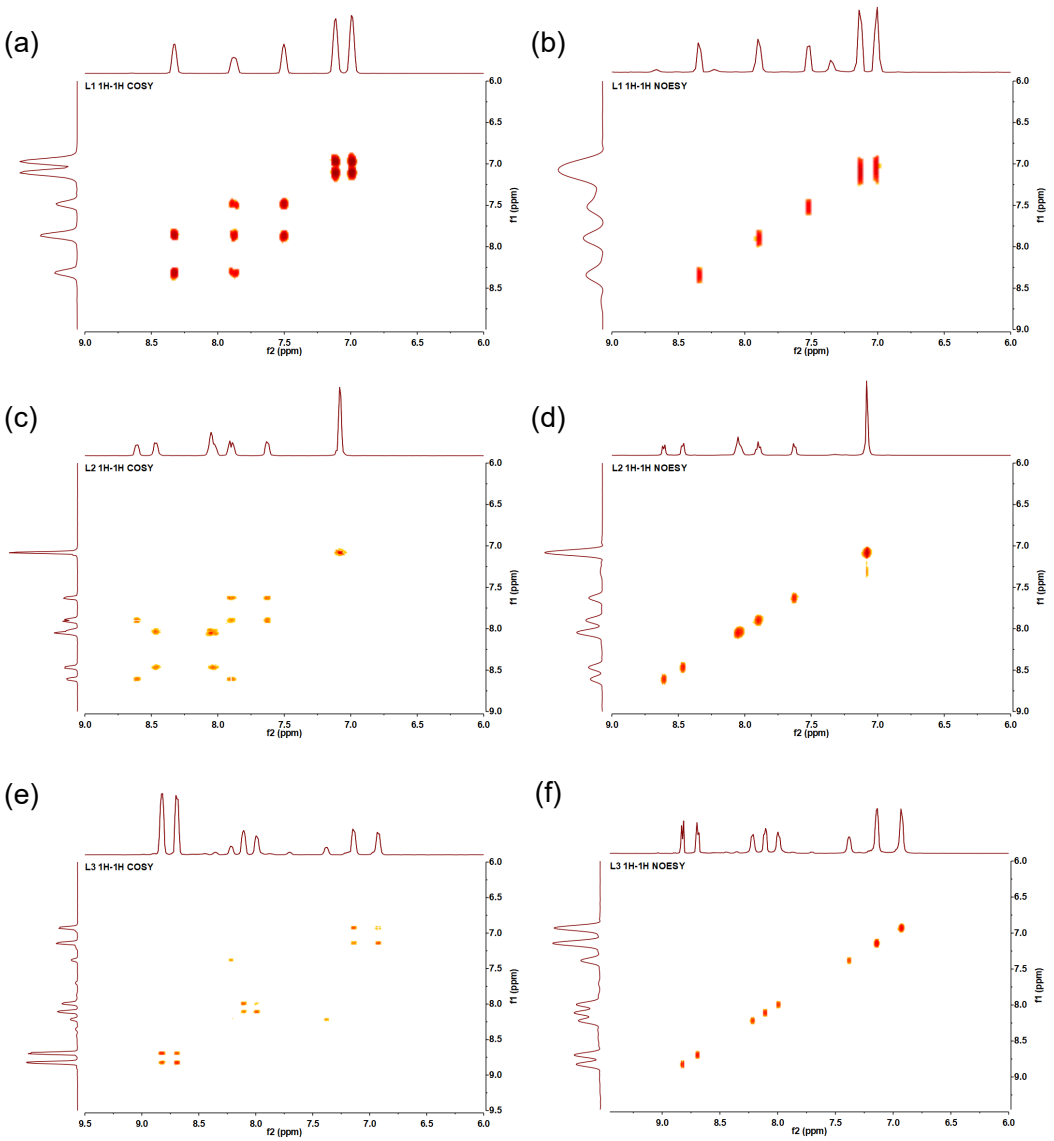


Figure S31. ^{1}H-^{1}H COSY spectrum of (a) **L1**, (c) **L2**, and **(**e) **L3;** ^{1}H-^{1}H NOESY spectrum of (b) **L1**, (d) **L2**, and **(**f) **L3**.

Table S8. Organic elements analysis of **L1**, **L2**, and **L3** extractants.

Extractant	Chemical formula	Element	C (%)	H(%)	N(%)
L1	$C_{26}H_{31}N_5O$	Prediction	72.70	7.27	16.30
		Measured	72.56	7.23	16.44
		Deviation	-0.136	0.03	0.14
L2	$C_{31}H_{34}N_6O$	Prediction	73.49	6.76	16.59
		Measured	73.44	6.74	16.72
		Deviation	-0.05	-0.02	0.13
L3	$C_{33}H_{34}N_6O$	Prediction	74.69	6.46	15.84
		Measured	74.64	6.15	15.82
		Deviation	-0.05	-0.31	-0.02

S 2.3 Extraction and Separation Performance

Table S9. The influence of solution acidity on the Ln(III) extraction by **L3** ([HNO_3] = 0.1-4.0 M, [L] = 20 mM).

Ln / Acidity	La	Ce	Pr	Nd	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
0.1	0.04	0.04	0.04	0.04	0.04	0.04	0.02	0.02	0.03	0.01	0.01	0.01	0.00	0.00
0.5	0.13	0.11	0.13	0.14	0.15	0.13	0.08	0.08	0.10	0.06	0.06	0.05	0.04	0.03
1.0	0.18	0.12	0.14	0.16	0.19	0.17	0.10	0.11	0.12	0.08	0.07	0.05	0.05	0.03
2.0	0.16	0.09	0.10	0.12	0.16	0.14	0.08	0.10	0.10	0.08	0.07	0.05	0.04	0.03
3.0	0.08	0.08	0.08	0.11	0.13	0.13	0.08	0.10	0.10	0.08	0.08	0.06	0.05	0.04
4.0	0.07	0.06	0.06	0.08	0.11	0.11	0.07	0.09	0.08	0.08	0.07	0.06	0.06	0.05

S 2.4 Coordination Modes in Solution

S 2.4.1 ^{1}H NMR titration spectra

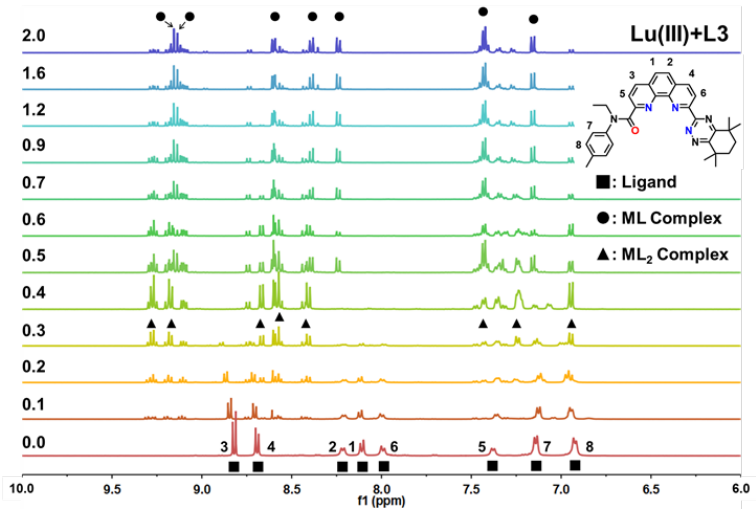


Figure S32. Stacked ^{1}H NMR titration spectra of Lu(III) and **L3** (■ = ligand peaks; ● = 1:1 complex peaks;

▲= 1:2 complex peaks).

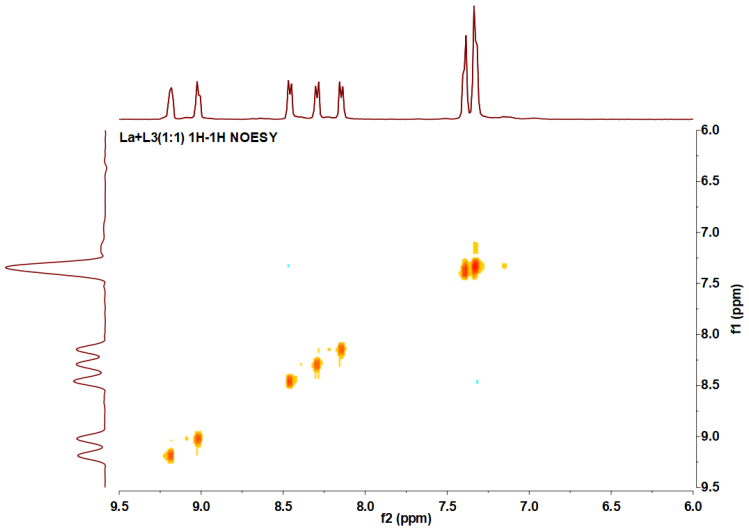


Figure S33. ^{1}H-^{1}H NOESY NMR spectra of La(III) and **L3** complex.

S 2.4.2 ESI-MS spectrum

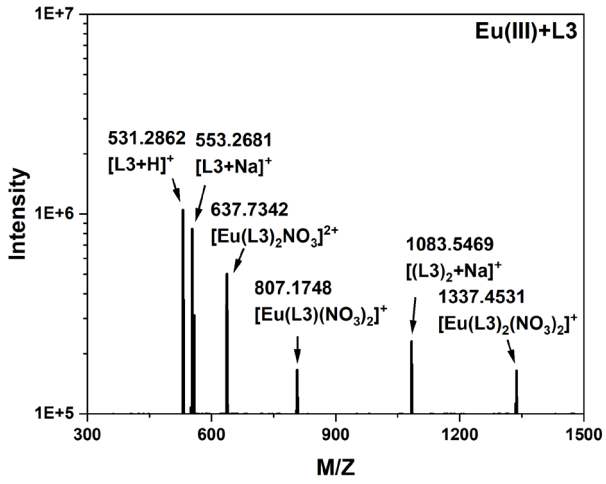


Figure S34. ESI-MS result of Eu(III) and **L3** complex.

*S 2.4.3 Simulated UV-vis spectra of **L3** and its Eu complexes*

In all tables within this part, the HOMO and LUMO are denoted as H and L, respectively. Alpha and beta orbitals are labelled with subscripts α and β, respectively.

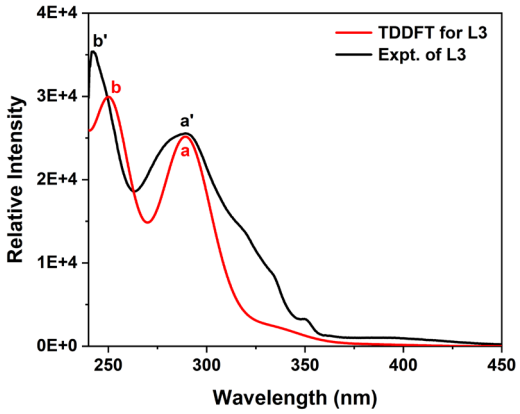


Figure S35. TDDFT/PBE0 simulated and experimental UV-vis spectra of **L3**. The calculated spectrum was blue-shifted by 2,229 cm^{-1} to align with the experimental absorption peaks at 34,578 cm^{-1} (289 nm), labelled as a'.

Table S10. Selected electronic excitations of **L3**, along with the oscillator strengths and transition types of the main absorption peaks. The analysis was based on the data from the peaks after the shift.

Peak	Energy at Peak maximum(nm)	Transition Energy(nm)	Oscillator Strength	Dominant Contributions		Assignment
				Occupied	Unoccupied	
a	289.2	291.8	2.0E-01	H-3	L	Ligand π → Ligand π*
		290.3	3.4E-02	H-4	L	Ligand π → Ligand π*
		287.2	9.5E-02	H-5	L	Ligand π → Ligand π*
		280.0	1.4E-02	H-1	L+2	Ligand N2p → Ligand π*
b	250.1	249.8	8.9E-02	H-4	L+2	Ligand π → Ligand π*
		246.1	1.1E-02	H-3	L+3	Ligand π → Ligand π*

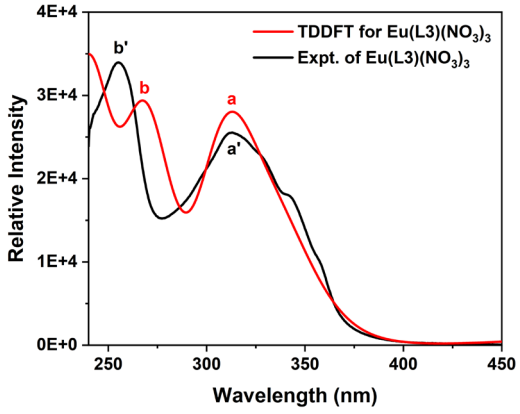


Figure S36. TDDFT/PBE0 simulated and experimental UV-vis spectra of Eu(**L3**)$(NO_3)_3$. The calculated spectrum was blue-shifted by 670 cm^{-1} to align with the experimental absorption peaks at 31,949 cm^{-1} (313nm), labelled as a'.

Table S11. Selected electronic excitations of Eu(**L3**)$(NO_3)_3$, along with the oscillator strengths and transition types of the main absorption peaks. The analysis was based on the data from the peaks after the shift.

Peak	Energy at Peak maximum(nm)	Transition Energy(nm)	Oscillator Strength	Dominant Contributions		Assignment
				Occupied	Unoccupied	
a	313.0	346.3	1.3E-02	Hα-6	Lα	Ligand π → Eu 4f
		336.1	1.4E-01	Hα-3	Lα+1	Ligand π + NO_3^- O2p → Ligand π*
		316.2	1.1E-01	Hα-5	Lα+1	Ligand π → Ligand π*
		308.9	2.3E-01	Hβ-3	Lβ+1	Ligand π + NO_3^- O2p → Ligand π*
b	267.4	269.6	9.4E-02	Hβ-13	Lβ	NO_3^- O2p → Ligand π*
		259.1	5.9E-03	Hα-23	Lα	Ligand π → Eu 4f

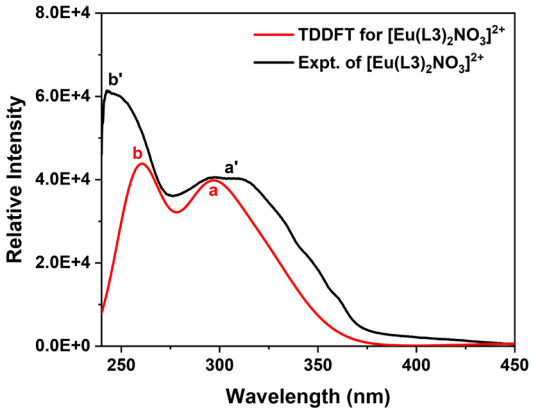


Figure S37. TDDFT/PBE0 simulated and experimental UV-vis spectra of $[Eu(\mathbf{L3})_2NO_3]^{2+}$. The calculated spectrum was blue-shifted by 3,491 cm^{-1} to align with the experimental absorption peaks at 33,670 cm^{-1} (297 nm), labelled as 'a'.

Table S12. Selected electronic excitations of $[Eu(\mathbf{L3})_2NO_3]^{2+}$, along with the oscillator strengths and transition types of the main absorption peaks. The analysis was based on the data from the peaks after the shift.

Peak	Energy at Peak maximum(nm)	Transition Energy(nm)	Oscillator Strength	Dominant Contributions		Assignment
				Occupied	Unoccupied	
a	297.0	305.9	9.0E-02	Hβ-3	Lβ	Ligand π + N2p → Ligand π*
		305.4	2.7E-02	Hα-15	Lα	Ligand π + NO_3^- O2p → Eu 4f
		300.9	7.1E-02	Hβ-4	Lβ	Ligand π → Ligand π*
		297.1	8.5E-02	Hβ-5	Lβ	Ligand π + N2p → Ligand π*
		294.3	9.9E-02	Hα-1	Lα+3	Ligand π → Ligand π*
b	260.5	262.8	4.9E-02	Hα-29	Lα	Ligand π + N2p →Eu 4f
		262.5	6.7E-02	Hβ-6	Lβ+2	Ligand π → Ligand π*

S 2.4.4 Theoretically predicted UV-vis spectra of Am complexes

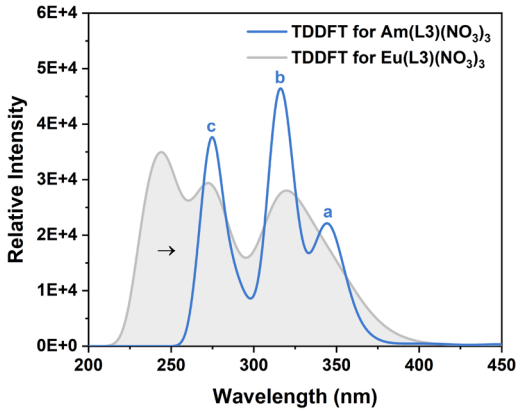


Figure S38. TDDFT/PBE0 simulated UV-vis spectra of Am(**L3**)$(NO_3)_3$ and Eu(**L3**)$(NO_3)_3$ complexes.

Table S13. Selected electronic excitations of Am(**L3**)$(NO_3)_3$, along with the oscillator strengths and transition types of the main absorption peaks.

Peak	Energy at Peak maximum(nm)	Transition Energy(nm)	Oscillator Strength	Dominant Contributions		Assignment
				Occupied	Unoccupied	
a	344.2	353.0	2.8E-02	Hβ-1	Lβ	Ligand π + NO_3^- O2p →Ligand π*
		346.9	4.9E-02	Hα-7	Lα	Ligand π + Am 5f →Ligand π*
		341.9	5.3E-02	Hβ-3	Lβ	NO_3^- O2p → Ligand π*
b	316.2	314.8	1.9E-01	Hβ-3	Lβ+1	NO_3^- O2p → Ligand π*
		313.8	5.9E-02	Hα-8	Lα+1	NO_3^- O2p + Am 5f → Ligand π*
c	274.8	275.5	9.0E-02	Hα-12	Lα+1	Ligand π → Ligand π*
		271.8	3.4E-02	Hα-11	Lα+2	Ligand π → Ligand π*

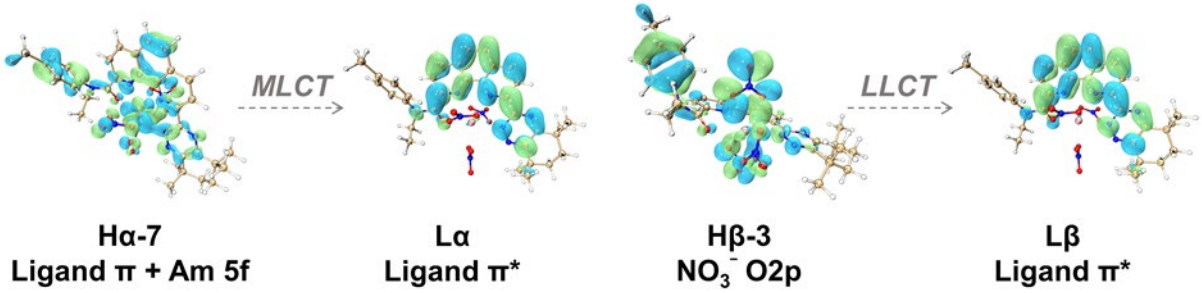


Figure S39. Dominant orbital character of Am(**L3**)$(NO_3)_3$ associated with electronic transitions. The contour value is 0.02 a.u.

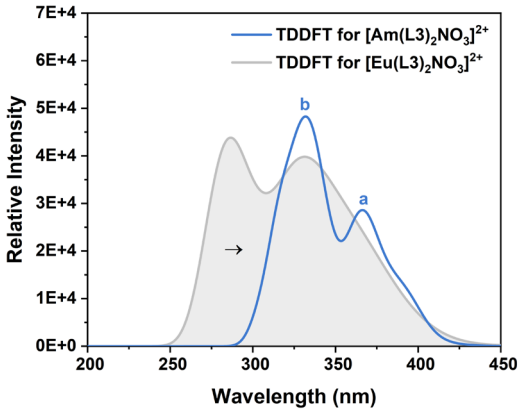


Figure S40. TDDFT/PBE0 simulated UV-vis spectra of $[Am(\mathbf{L3})_2NO_3]^{2+}$ and $[Eu(\mathbf{L3})_2NO_3]^{2+}$ complexes.

Table S14. Selected electronic excitations of $[Am(\mathbf{L3})_2NO_3]^{2+}$, along with the oscillator strengths and transition types of the main absorption peaks.

Peak	Energy at Peak maximum(nm)	Transition Energy(nm)	Oscillator Strength	Dominant Contributions		Assignment
				Occupied	Unoccupied	
a	366.2	365.5	4.6E-02	Hα-4	Lα+2	Am 5f → Ligand π*
		364.3	3.0E-02	Hα	Lα+3	Ligand π → Ligand π*
b	331.9	341.2	1.1E-01	Hβ-3	Lβ	Ligand π → Ligand π*
		336.8	5.1E-02	Hβ-1	Lβ+2	Ligand π → Ligand π*
		328.9	1.1E-02	Hα-9	Lα	NO_3^- O2p + Am 5f → Ligand π*
		320.8	2.1E-02	Hα-8	Lα+1	Ligand π + Am 5f → Ligand π*

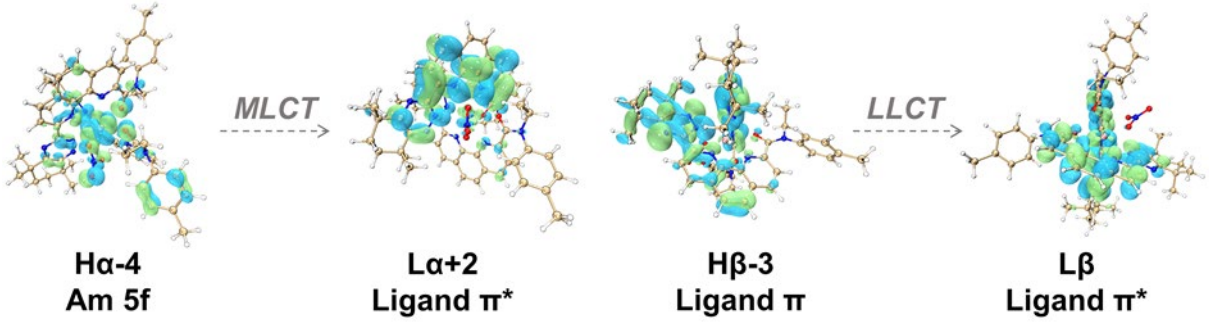


Figure S41. Dominant orbital character of $[Am(\mathbf{L3})_2NO_3]^{2+}$ associated with electronic transitions. The contour value is 0.02 a.u.

S 2.4.5 Photoluminescence Spectra Titration

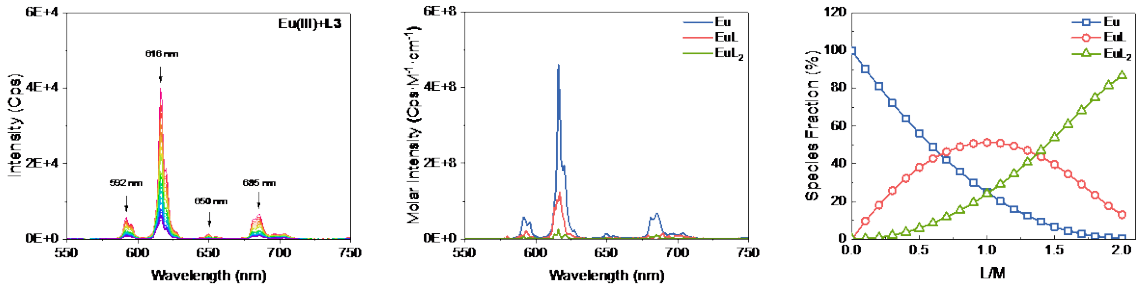


Figure S42. (a) Photoluminescence emission spectra of Eu(III) with **L3;** (b) Molar photoluminescence intensity of ligands and complexes of Eu(III) with **L3**; (c) Species fraction with increasing equivalents of Eu(III) with **L3** during photoluminescence titration.

Table S15. Complex reactions and fitted stability constants (log β) of **L3** with Eu(III) during UV-vis titration and photoluminescence titration.

Methods	Reaction	log β	Standard deviation	Ion
UV-vis titration	Eu^{3+}+**L3**→Eu(**L3**)$^{3+}$	6.41	0.02	0.01 M $Et_4N{\cdot}NO_3$
	Eu^{3+}+2**L3**→Eu(**L3**)$_2^{3+}$	11.73	0.05	
Photoluminescence titration	Eu^{3+}+**L3**→Eu(**L3**)$^{3+}$	6.61	0.03	
	Eu^{3+}+2**L3**→Eu(**L3**)$_2^{3+}$	11.87	0.06	

S 2.5 Complexes Structures in the Solid State

*S 2.5.1 Parameters of single crystals of **L3** complexes*

Table S16. The average bond length of different ligands with Eu(III) in complexes

Complex	Coordination Bond	Average bond length (Å) [a]
Eu(**L3**)$(NO_3)_3$	Eu-N(phen)	2.56 (2.62)
	Eu-N(triazine)	2.57 (2.57)
	Eu-O(amide)	2.40 (2.46)
	Eu-O(NO_3^-)	2.51 (2.50)
[Eu(**L3**)$_2$(ClO_4)](ClO_4)$_2$	Eu-N(phen)	2.53
	Eu-N(triazine)	2.57
	Eu-O(amide)	2.43
	Eu-O(ClO_4^-)	2.53

[a] The numbers in parentheses represent the calculated bond lengths. The difference between the experimental bond lengths and the calculated bond lengths is within 3%.

Table S17. Crystal data and structure refinement for **L3** extractant.

Name	**L3**
CCDC number	2348572
Empirical formula	$C_{35}H_{39}N_7O_2$
Formula weight	589.73
Temperature/K	170
Crystal system	monoclinic
Space group	P21/c
a/Å	12.6666(8)
b/Å	15.1869(11)
c/Å	17.3543(12)
α/°	90
β/°	104.941(4)
γ/°	90
Volume/Å^3	3225.5(4)
Z	4
ρ_{calc}g/cm^3	1.214
μ/mm^{-1}	0.619
F(000)	1256
Crystal size/mm^3	0.2 × 0.12 × 0.08
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	7.222 to 137.804
Index ranges	-15 ⩽ h ⩽ 12, -18 ⩽ k ⩽ 16, -20 ⩽ l ⩽ 20
Reflections collected	28945
Independent reflections	5925 [R_{int} = 0.0760, R_{sigma} = 0.0568]
Data/restraints/parameters	5925/18/407
Goodness-of-fit on F^2	1.09
Final R indexes [I>=2σ (I)]	R_1 = 0.0956, wR_2 = 0.2738
Final R indexes [all data]	R_1 = 0.1121, wR_2 = 0.2911
Largest diff. peak/hole / e Å^{-3}	0.66/-0.39

Table S18. Crystal data and structure refinement for Eu(**L3**)$(NO_3)_3$ and [Eu(**L3**)$_2(ClO_4)$]$(ClO_4)_2$.

Name	Eu(**L3**)$(NO_3)_3$	[Eu(**L3**)$_2(ClO_4)$]$(ClO_4)_2$
CCDC number	2348576	2348577
Empirical formula	$C_{35}H_{37}EuN_{10}O_{10}$	$C_{74}H_{84}Cl_3EuN_{14}O_{15}$
Formula weight	909.7	1667.86
Temperature/K	299	170.00
Crystal system	triclinic	triclinic
Space group	P-1	P-1
a/Å	9.0104(2)	16.0691(8)
b/Å	12.6375(3)	16.5029(7)
c/Å	17.6430(5)	16.9304(7)
α/°	87.428(2)	87.119(2)
β/°	86.868(2)	79.668(2)
γ/°	72.633(2)	62.539(2)
Volume/Å^3	1913.68(9)	3916.5(3)
Z	2	2
ρ_{calc}g/cm^3	1.579	1.414
μ/mm^{-1}	12.326	0.975
F(000)	920	1720.0
Crystal size/mm^3	0.15 × 0.1 × 0.08	0.23 × 0.1 × 0.07
Radiation	CuKα (λ = 1.54178)	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.018 to 136.726	4.09 to 55.07
Index ranges	-9 ⩽ h ⩽ 10, -15 ⩽ k ⩽ 15, -21 ⩽ l ⩽ 21	-20 ≤ h ≤ 20, -21 ≤ k ≤ 21, -22 ≤ l ≤ 21
Reflections collected	22978	74787
Independent reflections	6966 [R_{int} = 0.0648, R_{sigma} = 0.0601]	17912 [R_{int} = 0.0553, R_{sigma} = 0.0488]
Data/restraints/parameters	6966/72/512	17912/257/1064
Goodness-of-fit on F^2	1.059	1.118
Final R indexes [I>=2σ (I)]	R_1 = 0.0377, wR_2 = 0.0854	R_1 = 0.0562, wR_2 = 0.1231
Final R indexes [all data]	R_1 = 0.0531, wR_2 = 0.0936	R_1 = 0.0724, wR_2 = 0.1335
Largest diff. peak/hole / e Å^{-3}	0.60/-0.71	1.16/-0.98

S 2.5.2 The Most Stable Configuration of ML_2-type Complexes Using DFT

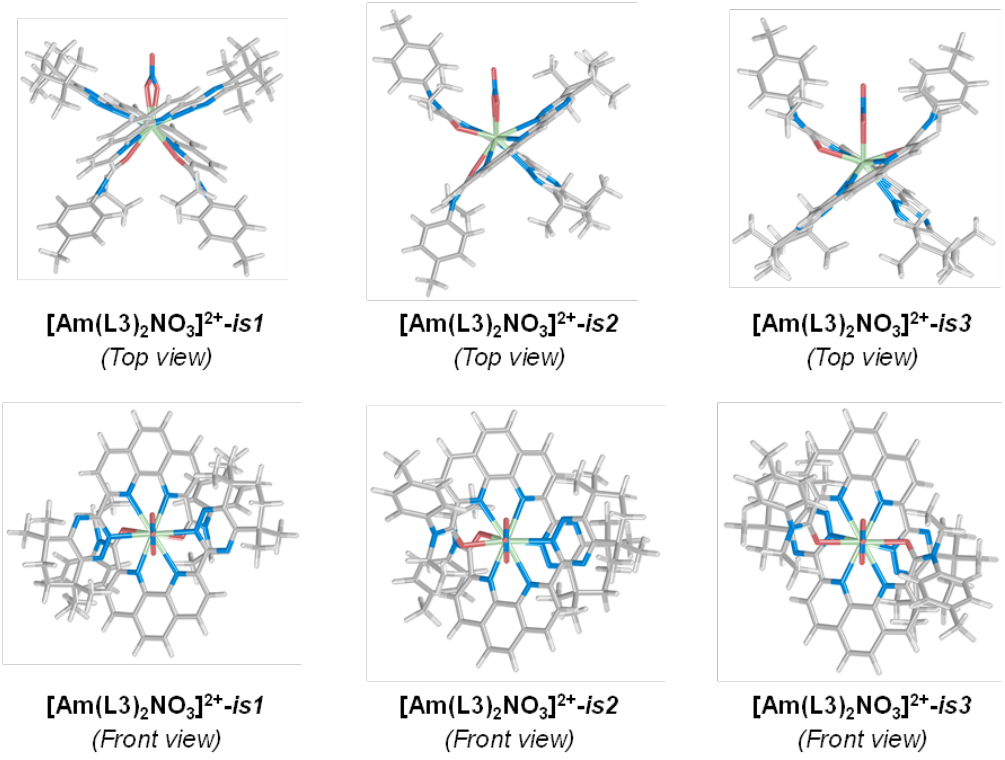


Figure S43. Optimized structures of three isomers of $[Am(\mathbf{L3})_2NO_3]^{2+}$ complexes (top views and front views). For *is1*, the nitrate ion is adjacent to two triazine side chains. For *is2*, the nitrate ion is adjacent to one amide side chain and one triazine side chain. For *is3*, the nitrate ion is adjacent to two amide side chains.

Table S19. Relative energies (in kcal/mol) of various isomers in the $[Am(\mathbf{L3})_2NO_3]^{2+}$ complexes.

Isomer	*is1*	*is2*	*is3*
ΔE	4.48	0	8.80

Due to the very small energy difference between isomer 1 and isomer 2 (0.11 kcal/mol), we further calculated the UV-vis spectra using TDDFT method for the three isomers (**Figure S45**). The results show that the spectrum of isomer 2 is closest to the experimental spectrum. Additionally, the relative position of the nitrate ion in the isomer 2 aligns with the relative position of perchlorate ion in the crystal $[Eu(\mathbf{L3})_2(ClO_4)](ClO_4)_2$. Based on these facts, we identify the isomer 2 as the actual configuration during the extraction process of the Eu(III) complexes.

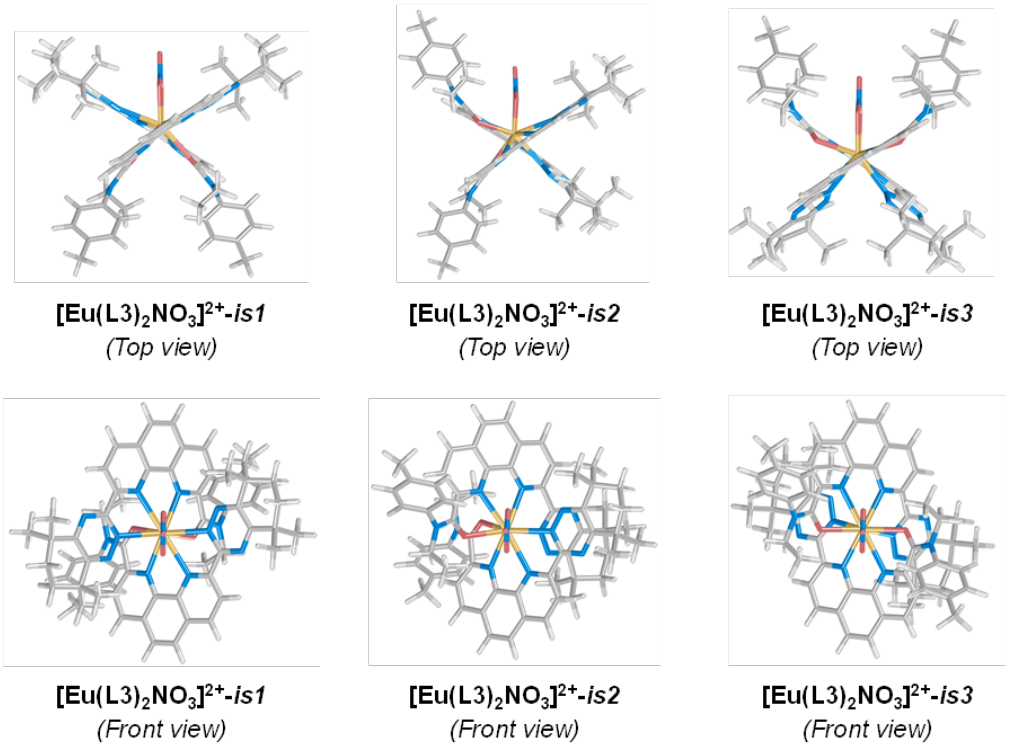


Figure S44. Optimized structures of $[Eu(\mathbf{L3})_2NO_3]^{2+}$ complex (top views and front views). The meanings of *is1* -*is3* are the same as in $[Am(\mathbf{L3})_2NO_3]^{2+}$ complex.

Table S20. Calculated relative Energies (ΔE in kcal/mol) of various isomers in the $[Eu(\mathbf{L3})_2NO_3]^{2+}$.

Isomer	*Is1*	*Is2*	*Is3*
ΔE	0	0.11	5.05

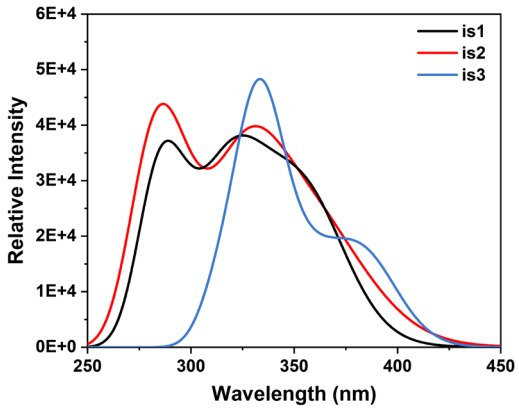
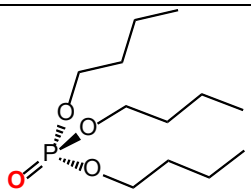
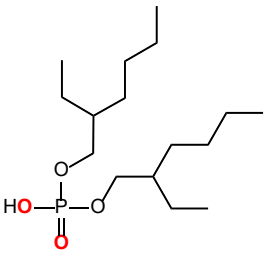
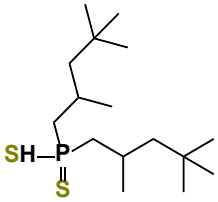
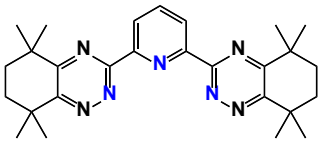
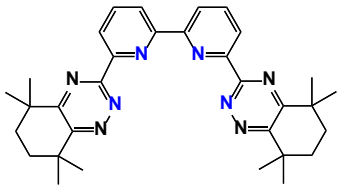
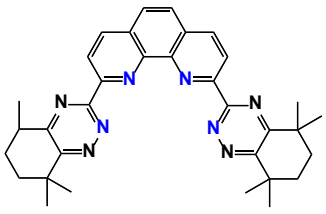
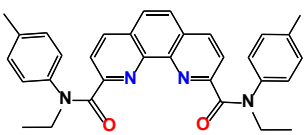
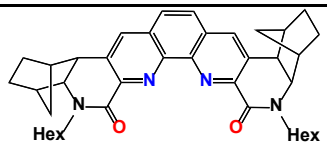
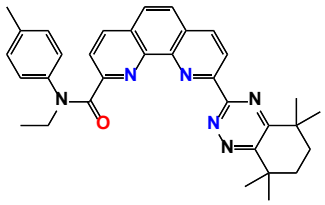


Figure S45. TDDFT/PBE0 simulated UV-vis spectra of three isomers of $[Eu(\mathbf{L3})_2NO_3]^{2+}$.

Appendix A

The advantages, disadvantages, and process of actinide/lanthanide separation extractants

Name	Chemical structure	Advantages	Disadvantages	Process and references
Neutral organophosphorus extractants (TBP)		High-valent actinides Extraction and separation.	Lack An(III)/Ln(III) separation ability.	PUREX [1]
Acidic organophosphorus extractants (HDEHP)		Medium separation factor ($SF_{Am(III)/Nd(III)}$ ≈100).	Hydrophilic masking agents (DTPA).	TALSPEAK [2, 3]
HBTMPDTP		High separation factor ($SF_{Am(III)/Eu(III)}$ ≈5900).	Low and narrow acidity; Poor structural stability.	TRANSDA [4-6]
BTP		Higher extraction acidity and medium separation ability (1 M HNO_3, $SF_{Am(III)/Eu(III)}$ ≈ 150).	Unsatisfied acidic and radio stability.	SANEX [7, 8]
BTBP		Proved radiolysis resistance.	Slow extraction rate.	1-cycle SANEX [9]
BTPhen		Good Am(III) extraction ability $D_{Am(III)} > 1000$, $SF_{Am(III)/Eu(III)} > 200$, $T_{Am(III)} \approx 15$ min).	Difficult Am(III) stripping.	/ [10]
DAPhen		Good An(III/IV/VI)/Ln(III) separation ($D_{Am(III)}$ ≈ 20, $D_{U(VI)} > 100$, $D_{Pu(IV)} > 300$).	Light Ln(III) coextraction	GANEX [11, 12]

BLPhen		Strong Am(III) extraction ($D_{Am(III)}$ > 1000).	All Ln(III) coextraction	/ [13, 14]
ATPhen		Good Am(III) extraction and stripping; all Ln(III) separation ($D_{Am(III)} \approx$ 40, $SF_{Am(III)/Ln(III)}$ > 280, $S_{Am(III)}$ > 92%).	/	In preparing This work

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[14] Healy M, Ivanov A, Karslyan Y, et al. Efficient Separation of Light Lanthanides(III) by Using Bis-Lactam Phenanthroline Ligands. *Chem. Eur. J.,* **2019**, 25, 6326-6331.

Appendix B

Cartesian coordinates of PBE0 optimized geometries of ligands and metal complexes.

Ligand 1-C1				Ligand 1-C2			
N	-1.58987000	1.16675800	-0.28164600	N	-0.61632100	-1.05313100	-0.02603800
N	0.70346400	-0.07011900	-1.10824000	N	1.44949000	0.70658600	-0.31288000
N	1.78035900	-0.76907100	-1.36098000	N	2.43402600	1.56920400	-0.30040500
N	1.94026100	1.34626200	0.31556500	N	2.95519000	-1.04553400	0.16609200
C	-0.34012900	2.93158500	0.72829600	C	0.87038200	-2.90486300	-0.25886700
C	0.80681700	0.94633200	-0.25386900	C	1.73751300	-0.57221000	-0.08175800
C	-1.50790000	3.62719000	0.99044000	C	-0.20595400	-3.77544600	-0.30346000
C	2.94256200	-0.46438200	-0.79342400	C	3.67968700	1.17890300	-0.05418200
C	-0.42781800	1.70577400	0.07199400	C	0.61594800	-1.54441100	-0.11848300
C	3.03454500	0.65797200	0.04453800	C	3.94892600	-0.17590400	0.20284200
C	-4.01014800	1.27268400	-0.50942500	C	-3.04500000	-1.37627100	0.16260700
C	-2.70167600	1.83526200	-0.01969800	C	-1.64126700	-1.88918500	-0.06262300
H	0.62944900	3.31755400	1.01187200	H	1.89148800	-3.25470600	-0.32836900
H	-1.47263600	4.58965200	1.48819100	H	-0.04434700	-4.84154800	-0.41549500
C	4.26502100	0.78856400	2.17671700	C	5.82337900	-1.46311200	-0.74599800
H	5.16485600	1.15659600	2.67667200	H	6.80490100	-1.90286300	-0.55063400
H	4.19037700	-0.28602500	2.35684200	H	5.90978300	-0.80951800	-1.61665900
H	3.39571900	1.26635500	2.63242600	H	5.12931900	-2.26745000	-0.99735200
C	4.47594500	2.63314200	0.51793000	C	5.27927200	-1.68295000	1.67437300
H	4.47898900	2.91895800	-0.53702400	H	4.89604300	-1.19392800	2.57353100
H	5.42121700	2.95897700	0.95985700	H	6.28502700	-2.05177100	1.89196800
H	3.66112100	3.16279200	1.01176000	H	4.63605600	-2.53425300	1.45171600
C	4.51007100	-1.08924400	-2.59906100	C	4.55854900	3.09433800	1.23079900
H	5.32353300	-1.75733800	-2.89477600	H	5.27892800	3.91668600	1.24466600
H	4.84242200	-0.05973000	-2.75076400	H	4.70681500	2.49606900	2.13271000
H	3.65808100	-1.26671500	-3.25779500	H	3.55199200	3.51499600	1.26965000
C	3.70650900	-2.82684100	-1.00830200	C	4.55041000	3.18448300	-1.25686500
H	4.55973200	-3.46843500	-1.24480300	H	5.32772900	3.95337400	-1.25390600
H	2.88726200	-3.06794500	-1.68550600	H	3.57541500	3.67061000	-1.23565900
H	3.38389300	-3.05401300	0.01124700	H	4.63077400	2.62490200	-2.19245300
C	4.32905200	1.12067300	0.68061100	C	5.33543900	-0.70926900	0.49779500
C	4.11382500	-1.35929400	-1.14255100	C	4.73414100	2.26645500	-0.04836100
C	5.28172100	-1.06685000	-0.19502500	C	6.12733300	1.63111600	-0.10134000
C	5.51559900	0.41734000	0.01386300	C	6.27644400	0.45037900	0.83905500
H	6.18353200	-1.54138500	-0.59364900	H	6.87089500	2.39894200	0.13275400
H	5.08662200	-1.54848200	0.76930100	H	6.33365300	1.31295900	-1.12900100
H	5.71693800	0.89742000	-0.94983000	H	6.08345400	0.77211200	1.86803200
H	6.40781400	0.58067300	0.62602500	H	7.30606200	0.08010600	0.82564500
C	-2.71634200	3.08265000	0.59703700	C	-1.48659400	-3.26830400	-0.19244500
H	-3.65890000	3.59424600	0.74238400	H	-2.36238300	-3.90329200	-0.18357200

O	-4.85960100	2.04007900	-0.93281100	O	-3.79695300	-2.09336800	0.80033700
C	-3.40733300	-0.97693500	0.26322400	C	-4.69705400	0.35329700	-0.00120800
C	-3.35015000	-0.83911900	1.64276000	C	-5.14207000	0.35395200	1.31884700
C	-2.74718700	-2.04242700	-0.33770200	C	-5.51181300	0.91382800	-0.97658800
C	-2.62204500	-1.73956100	2.40639700	C	-6.36972400	0.89971100	1.64070000
H	-3.87881200	-0.02093500	2.11927600	H	-4.52199700	-0.07853500	2.09182000
C	-2.03935700	-2.94495400	0.43333500	C	-6.74016500	1.46438700	-0.63942800
H	-2.76074500	-2.13862100	-1.41640700	H	-5.19490100	0.92186500	-2.01219900
H	-2.58053400	-1.61122200	3.48333500	H	-6.69181400	0.89204900	2.67744200
C	-1.95918300	-2.81019900	1.81871300	C	-7.19677200	1.46511200	0.67126700
H	-1.51705600	-3.76196900	-0.05421300	H	-7.35674900	1.89637800	-1.42117700
C	-1.19380700	-3.80119400	2.64277700	C	-8.53097500	2.04134700	1.03693000
H	-0.21086100	-4.00211200	2.20960200	H	-8.98631200	2.55666800	0.18974700
H	-1.72194200	-4.75786200	2.70104400	H	-8.44382700	2.75621500	1.85937000
H	-1.04775500	-3.44163200	3.66257800	H	-9.22337800	1.25911100	1.36210800
C	-5.38546100	-0.58662900	-1.17015500	C	-2.61737700	0.58542700	-1.31976300
C	-5.28392100	-0.60420200	-2.68389200	C	-2.57563400	-0.05375700	-2.69693400
H	-5.55585800	-1.59071600	-0.77994700	H	-3.06450400	1.57750100	-1.37853800
H	-6.22432000	0.04427000	-0.86495300	H	-1.60795900	0.70756900	-0.93099200
H	-6.21632800	-0.97717600	-3.11485800	H	-2.00207400	0.57944300	-3.37823400
H	-5.11176200	0.40239900	-3.06637100	H	-2.08836100	-1.03069500	-2.66644100
H	-4.47062300	-1.24959600	-3.02208200	H	-3.57429700	-0.19161200	-3.11725300
N	-4.18019200	-0.07563500	-0.51614400	N	-3.41409200	-0.16037900	-0.33639600
Ligand 1-C3				**Ligand 2-C1**			
N	-1.41154400	1.33642800	-0.11264700	C	-0.37121800	-1.31904000	-0.24014500
N	1.86140200	2.01785600	1.14709000	N	0.78894600	-0.69892100	-0.42089400
N	3.09184200	1.57872400	1.07451000	C	1.88384200	-1.20848200	0.12947700
N	1.17885900	0.48643800	-0.50938500	C	1.86548500	-2.37216500	0.89505600
C	-0.63665900	3.25282400	1.08666500	C	0.65475000	-3.01867200	1.07797500
C	0.94598600	1.47286300	0.34724200	C	-0.48743500	-2.49249200	0.50518500
C	-1.91883900	3.77228600	1.11444800	C	-1.56032700	-0.70747600	-0.88227100
C	3.41113200	0.60581500	0.22933100	N	-2.74003600	-1.26715300	-0.62312300
C	-0.42575400	2.03576200	0.44120300	C	-3.82534600	-0.74171900	-1.17355200
C	2.41373400	0.02357700	-0.57213500	C	-3.78869600	0.35951300	-2.02032600
C	-3.74001400	1.10072400	-0.78060000	C	-2.55704300	0.92665600	-2.30326300
C	-2.63672600	1.83856100	-0.07022800	C	-1.42051300	0.39434700	-1.72449400
H	0.20014500	3.76546800	1.54114700	H	2.78456300	-2.74601400	1.32456200
H	-2.11421000	4.72444300	1.59445800	H	0.60479600	-3.93092200	1.66190300
C	2.61788700	-0.52149100	-2.96363700	H	-1.45825900	-2.95806500	0.61066000
H	2.75399700	-1.31965000	-3.69818600	H	-4.70293100	0.75511600	-2.44505700
H	3.38931500	0.23299200	-3.13341200	H	-2.48556800	1.77909000	-2.96946400
H	1.64609700	-0.05462000	-3.13418700	H	-0.43273300	0.79911000	-1.90225800
C	1.59500300	-2.17111200	-1.40539800	N	4.27689700	1.19022700	-1.13189900

H	1.58677300	-2.59390300	-0.39731900
H	1.78447800	-2.98226200	-2.11369300
H	0.60897700	-1.74995800	-1.60129500
C	5.13894800	-0.61538100	1.50389900
H	6.19232400	-0.90564200	1.54504200
H	4.53270100	-1.52182100	1.56812300
H	4.91489900	0.00028100	2.37707800
C	5.77584400	1.40059900	0.19034100
H	6.82067900	1.07950800	0.16236500
H	5.62358100	2.02341000	1.07158500
H	5.58563400	2.01254800	-0.69520600
C	2.68073100	-1.10492300	-1.54614300
C	4.86324100	0.17439200	0.21859600
C	5.13188100	-0.68596200	-1.02050200
C	4.05345100	-1.72417300	-1.26676100
H	6.10668500	-1.16976300	-0.90554000
H	5.21934800	-0.03126200	-1.89436300
H	3.97427400	-2.38627900	-0.39776800
H	4.32700000	-2.36442200	-2.11101000
C	-2.94196300	3.06597600	0.50880200
H	-3.95709100	3.43903200	0.46546300
O	-4.55079900	1.74007600	-1.43016700
C	-3.10705300	-1.02905200	0.26300000
C	-3.21576700	-0.70606700	1.61070500
C	-2.38842200	-2.16288300	-0.09710400
C	-2.58743500	-1.48172100	2.57055200
H	-3.79758500	0.15878200	1.90820500
C	-1.78316700	-2.94430800	0.87171400
H	-2.28608100	-2.42149600	-1.14434200
H	-2.67649200	-1.20434000	3.61611000
C	-1.86402500	-2.61808700	2.22266600
H	-1.22063600	-3.82160800	0.56811000
C	-1.22283700	-3.47895700	3.26873800
H	-0.36212500	-4.01758400	2.86775700
H	-1.92667800	-4.22597900	3.64954400
H	-0.88571100	-2.88578700	4.12099600
C	-4.73296700	-0.92897800	-1.59949100
C	-4.28818900	-0.98651600	-3.04892400
H	-4.88482000	-1.93110300	-1.19729700
H	-5.67964200	-0.38755100	-1.52795200
H	-5.05278800	-1.48109600	-3.65292800
H	-4.14268400	0.01952500	-3.44362000
H	-3.35440200	-1.54187500	-3.16026100
N	-3.77023000	-0.25961900	-0.72358700
N	3.16055300	0.52975500	-0.95809000
C	5.38237600	0.84851000	-0.47923400
C	6.60882500	1.69592200	-0.74831300
C	7.68930800	1.37717800	0.29010900
C	7.85292500	-0.11077900	0.53568600
C	6.59373000	-0.76263300	1.11586600
C	5.36999300	-0.26664600	0.37358300
N	4.23575300	-0.91574600	0.56315400
C	3.16375200	-0.48711000	-0.09786000
C	6.42375700	-0.40385800	2.59754600
H	7.26840400	-0.79310800	3.17216200
H	6.37190900	0.67542300	2.75643700
H	5.50562800	-0.84522200	2.98987000
C	6.70017800	-2.28159400	0.98600400
H	6.77692100	-2.58437000	-0.06139300
H	7.59554000	-2.63171800	1.50635700
H	5.83067400	-2.77563800	1.41973400
C	7.10482100	1.38837200	-2.16635100
H	6.31318100	1.58748000	-2.89096400
H	7.96353600	2.02100200	-2.40701800
H	7.40787700	0.34491500	-2.27917100
C	6.24742600	3.17915800	-0.66515400
H	5.85639900	3.43440900	0.32323100
H	7.13982900	3.78525200	-0.84368800
H	5.49187100	3.43948900	-1.40618700
H	7.43831500	1.88052700	1.23008300
H	8.63562600	1.81353500	-0.04374100
H	8.68807600	-0.29518700	1.21834100
H	8.11196300	-0.61257300	-0.40286200
C	-5.11319200	-1.48585400	-0.92278200
O	-5.20283700	-2.66107900	-1.21420800
N	-6.17256500	-0.76677400	-0.44011100
C	-6.03136700	0.49106400	0.20007500
C	-5.11298300	0.67429400	1.22740300
C	-6.84136400	1.55913800	-0.17346600
C	-4.99045000	1.90929600	1.84415400
H	-4.49157000	-0.15633000	1.54140900
C	-6.72307000	2.78326100	0.46100100
H	-7.56157600	1.43123900	-0.97406100
H	-4.26360900	2.03230000	2.64052900
H	-7.36454100	3.60345200	0.15459900
C	-5.63975900	4.32502500	2.13104700
H	-6.59717600	4.84510100	2.20069800
H	-4.96125400	4.96617300	1.55946200

			H	-5.22887400	4.23103500	3.13770500
			C	-5.79015400	2.98586800	1.47567100
			C	-7.45411600	-1.45807200	-0.32490600
			C	-7.61960300	-2.17221700	1.00390900
			H	-7.50603900	-2.17297600	-1.14584500
			H	-8.24508900	-0.71822800	-0.46317800
			H	-8.59766000	-2.65677100	1.05189400
			H	-6.85209100	-2.93891000	1.11989400
			H	-7.54746600	-1.47246100	1.83997200
Ligand 2-C2			**Ligand 2-C3**		
C	-0.11452000	-0.11492600	-0.40632200	C	0.26525700	-1.64250600	-0.03895800
N	1.15462600	0.26146000	-0.30134700	N	-0.95880900	-1.12678000	0.00552300
C	2.10709700	-0.66131100	-0.34350300	C	-1.94545400	-1.76122600	-0.61565900
C	1.82932600	-2.01837600	-0.49256700	C	-1.75170600	-2.95131200	-1.31469900
C	0.50583500	-2.40806500	-0.60653100	C	-0.47613100	-3.48672100	-1.35452100
C	-0.48871700	-1.44927300	-0.56464000	C	0.55522800	-2.83000100	-0.70969700
C	-1.13201500	0.96309000	-0.35405600	C	1.33241000	-0.89670100	0.67230500
N	-2.41226500	0.59051400	-0.34596500	N	2.57323800	-1.36585800	0.55958500
C	-3.34919700	1.53015900	-0.32986600	C	3.55472800	-0.71938800	1.17227700
C	-3.05482100	2.88934500	-0.32200400	C	3.34961900	0.42140500	1.93866700
C	-1.72514000	3.27211700	-0.29628900	C	2.05491000	0.89552500	2.07051000
C	-0.74212700	2.29942800	-0.31560100	C	1.02613600	0.23484500	1.42628000
H	2.64083900	-2.73226200	-0.51880700	H	-2.59136400	-3.42629400	-1.80292300
H	0.25318800	-3.45513000	-0.73102700	H	-0.28929200	-4.41419500	-1.88404200
H	-1.53710800	-1.69981500	-0.65452500	H	1.56948700	-3.20614900	-0.70354500
H	-3.86141300	3.61001800	-0.35271100	H	4.18430100	0.91766700	2.41796100
H	-1.45620100	4.32219400	-0.27443100	H	1.85192100	1.77571400	2.67034100
H	0.31334500	2.53835900	-0.30774200	H	-0.00319500	0.56239200	1.48670800
N	4.97363500	1.52656200	-0.09096200	N	-5.48210700	-1.29869900	-1.14286300
N	3.73993300	1.11442400	-0.23517800	N	-4.26671900	-1.77666400	-1.21023300
C	5.97155400	0.66093300	0.04966400	C	-5.73887300	-0.20731600	-0.43121400
C	7.35354300	1.25478800	0.22784300	C	-7.18077100	0.25625100	-0.40859600
C	8.32686100	0.16060500	0.67805600	C	-7.36317200	1.30385500	0.69444400
C	8.16675200	-1.13060200	-0.10174000	C	-6.25452200	2.33920000	0.71663200
C	6.78996300	-1.77566400	0.08713800	C	-4.87932900	1.73522900	1.01697700
C	5.71017400	-0.71753400	-0.00662800	C	-4.68855800	0.46065500	0.22102600
N	4.46094900	-1.12812200	-0.12910700	N	-3.46837200	-0.04117200	0.16837000
C	3.51488500	-0.19794200	-0.22395800	C	-3.29949500	-1.15161500	-0.53956100
C	6.68052400	-2.44046200	1.46515200	C	-4.74682100	1.38148400	2.50377000
H	7.41483700	-3.24618200	1.54680700	H	-4.82339900	2.28918300	3.10824700
H	6.85834700	-1.73363800	2.27847900	H	-5.52292300	0.68673800	2.83249300
H	5.68421500	-2.86526800	1.60153600	H	-3.77734700	0.91748900	2.69432100
C	6.57227700	-2.83698300	-0.99069700	C	-3.78586000	2.73825500	0.65068700

H	6.59648400	-2.39597200	-1.99045700	H	-3.82602900	2.99518000	-0.41105800
H	7.36584500	-3.58648300	-0.93185700	H	-3.92320100	3.65703600	1.22707400
H	5.61210500	-3.33698000	-0.86279300	H	-2.79704100	2.33208700	0.86375800
C	7.79296900	1.86168900	-1.11012200	C	-7.51927500	0.84436800	-1.78379400
H	7.07205200	2.61435300	-1.43438500	H	-7.35469000	0.09645000	-2.56168700
H	8.76957900	2.34073400	-0.99968900	H	-8.56908700	1.14878700	-1.81159200
H	7.86962900	1.10916200	-1.89830900	H	-6.90518900	1.71601900	-2.02130200
C	7.31371800	2.36286300	1.28057300	C	-8.10820100	-0.92909100	-0.13959900
H	6.97105400	1.97818000	2.24470200	H	-7.87644500	-1.40082800	0.81884700
H	8.31697400	2.77551100	1.41739900	H	-9.14500600	-0.58349200	-0.10543700
H	6.64198200	3.16586700	0.97776100	H	-8.01556100	-1.68410600	-0.92006700
H	8.17571700	-0.03223400	1.74569000	H	-7.41115000	0.79441100	1.66302800
H	9.34881400	0.53927100	0.58054000	H	-8.33449900	1.78924600	0.55887600
H	8.93426300	-1.85248500	0.19366400	H	-6.46846300	3.11068800	1.46265500
H	8.32535900	-0.93879500	-1.16840200	H	-6.21292700	2.85478000	-0.24886400
C	-4.80213100	1.13653900	-0.45248900	C	4.91594400	-1.36462000	1.09163800
O	-5.48353200	1.74800600	-1.25563700	O	5.07255300	-2.50155100	1.48774300
N	-5.29059600	0.11860500	0.31163100	N	5.95195900	-0.59504400	0.63861600
C	-6.65129300	-0.27474000	0.13334900	C	5.76632200	0.59686800	-0.10781200
C	-7.69652500	0.62428100	0.30370400	C	4.93214300	0.62506300	-1.21939100
C	-6.93967600	-1.59353500	-0.18547100	C	6.45006800	1.75573500	0.24713200
C	-9.00592400	0.20139500	0.15670100	C	4.76609100	1.79747000	-1.93959700
H	-7.47821400	1.65818000	0.53770700	H	4.41122900	-0.27718200	-1.51818700
C	-8.25502800	-2.00977300	-0.32315400	C	6.29082500	2.91629900	-0.48950500
H	-6.12788600	-2.29678700	-0.33567000	H	7.10360200	1.74853200	1.11250000
H	-9.81137200	0.91647900	0.29157200	H	4.10682500	1.79896100	-2.80157500
H	-8.46188000	-3.04543100	-0.57292000	H	6.83398800	3.80913400	-0.19640800
C	-10.73290700	-1.55984300	-0.33896900	C	5.24242400	4.23356100	-2.36174200
H	-10.82289900	-2.64636800	-0.29375200	H	6.15912100	4.82552700	-2.39682700
H	-11.12224300	-1.23612000	-1.30917500	H	4.47012800	4.85591200	-1.89869500
H	-11.38228700	-1.13257900	0.42853000	H	4.92749900	4.03192300	-3.38698600
C	-9.31124400	-1.12091000	-0.15829100	C	5.43981900	2.96332800	-1.59163500
C	-4.60370600	-0.44713000	1.47066200	C	7.29016700	-1.17911900	0.68330000
C	-5.01455000	0.21276100	2.77501300	C	7.62668500	-1.97324300	-0.56533900
H	-3.53243900	-0.36466900	1.31000500	H	7.32799000	-1.82357500	1.56136600
H	-4.83738300	-1.51393000	1.50260300	H	8.00402500	-0.36499400	0.82365500
H	-4.51252200	-0.27164000	3.61606600	H	8.64090600	-2.37335900	-0.49531200
H	-4.73976900	1.27039500	2.78035300	H	6.93615200	-2.81019400	-0.67940000
H	-6.09244600	0.13836000	2.93509100	H	7.57123600	-1.34676100	-1.45880200
Ligand 3-C1				**Ligand 3-C2**			
N	1.65302500	0.44866300	0.08175000	N	1.95950900	-0.35939400	-0.82521700
N	2.59176900	1.34715800	-0.07290100	N	2.54559900	-1.52834300	-0.86480400
N	3.25767700	-1.27290400	-0.06300900	N	3.85335300	0.57229400	0.22801600

C	2.00652900	-0.83544200	0.04584900	C	2.61299600	0.64481400	-0.24490500
C	3.85889400	0.98938700	-0.25318800	C	3.75837900	-1.70249100	-0.34988500
C	-4.28418600	1.03074000	-1.59480000	C	-4.23682600	0.67087900	0.17532400
C	4.21071900	-0.36858600	-0.20401800	C	4.45571200	-0.60316900	0.17531200
C	5.79582600	-1.51587600	-1.70217700	C	5.80587800	-0.58494300	2.23699800
H	6.80250900	-1.93027700	-1.80178700	H	6.81733000	-0.59494400	2.65167700
H	5.63896300	-0.80263400	-2.51413500	H	5.24644500	-1.40991200	2.68313700
H	5.07419700	-2.32590100	-1.82331700	H	5.32014100	0.34743100	2.53077200
C	5.91106200	-1.91705100	0.75223000	C	6.70116500	0.47406300	0.16952000
H	6.94740000	-2.25629300	0.67581800	H	7.72645900	0.39461900	0.54017600
H	5.25448600	-2.77936700	0.63517100	H	6.28973900	1.43128900	0.49031800
H	5.76222700	-1.50709100	1.75451000	H	6.73461500	0.46424400	-0.92299600
C	5.63640100	-0.86542500	-0.32206200	C	5.87063900	-0.69031400	0.70799300
C	6.18977200	1.53941500	-0.92888400	C	5.57631500	-3.20130900	0.45149500
C	6.60946000	0.30562800	-0.15253100	C	6.50642600	-2.01570600	0.27654900
H	6.95425000	2.31801700	-0.84779900	H	6.09861100	-4.13275900	0.21313100
H	6.11601900	1.29690900	-1.99444800	H	5.27625700	-3.28237200	1.50178200
H	6.68917400	0.54976800	0.91231800	H	6.81145300	-1.93833000	-0.77267000
H	7.60641200	-0.02047300	-0.46419500	H	7.42661800	-2.16469100	0.84966100
O	-5.00805000	1.18381000	-2.56621400	O	-5.27305000	0.72839300	0.81935900
N	-3.60121900	2.04482300	-1.00971200	N	-3.78883000	-0.48268300	-0.38481900
C	-3.05730400	1.97168200	0.30602700	C	-4.51966200	-1.67493800	-0.10065100
C	-3.90298300	1.92490800	1.40458600	C	-4.61594000	-2.15380700	1.20032200
C	-1.68211700	1.98373300	0.50354100	C	-5.12201500	-2.38542700	-1.12693100
C	-3.37755600	1.88739200	2.68920900	C	-5.30170300	-3.32535800	1.46106000
H	-4.97661400	1.91552700	1.25116800	H	-4.15679900	-1.59465100	2.00610400
C	-1.16858400	1.95476600	1.78558000	C	-5.80244600	-3.56416200	-0.85701800
H	-1.01313700	1.95863500	-0.34750300	H	-5.07024700	-2.01162700	-2.14331900
H	-4.05069300	1.84454900	3.53956300	H	-5.36857300	-3.68386300	2.48357300
H	-0.09161700	1.93309300	1.91303600	H	-6.27015500	-4.10620600	-1.67263900
C	-1.43042400	1.88194500	4.28570700	C	-6.64126500	-5.32726600	0.73500900
H	-0.93244700	2.82626000	4.52501700	H	-7.07672700	-5.75401300	-0.16976100
H	-0.68376300	1.09017900	4.38791200	H	-7.45089000	-5.15828800	1.45022500
H	-2.20555600	1.71484600	5.03535800	H	-5.97608700	-6.07718600	1.17255400
C	-2.00479400	1.90931600	2.90119800	C	-5.90544200	-4.05550200	0.43827200
C	-3.63811900	3.35418400	-1.65148500	C	-2.62495300	-0.63217800	-1.25988400
C	-4.78578600	4.22764800	-1.17789200	C	-1.44804900	-1.28169500	-0.56338700
H	-3.71704900	3.18189500	-2.72526300	H	-2.34364200	0.34651900	-1.63766500
H	-2.67937300	3.83791500	-1.44882200	H	-2.94116000	-1.23615800	-2.11526000
H	-4.74919800	5.19872600	-1.67765500	H	-0.62177900	-1.41759500	-1.26296700
H	-5.74277100	3.75876800	-1.41326800	H	-1.08873000	-0.63753700	0.23930800
H	-4.73270800	4.40097700	-0.10064600	H	-1.72452300	-2.25739900	-0.15583700
C	4.85114600	2.11573600	-0.45592600	C	4.31929700	-3.10770200	-0.41942400
C	4.32080400	3.09419600	-1.50443400	C	3.27754800	-4.10805600	0.08287500

C	5.01607400	2.85996600	0.87455500	C	4.64348200	-3.42661600	-1.88381200
H	3.37708900	3.53615100	-1.18501700	H	2.37761100	-4.07706200	-0.53119400
H	4.15537000	2.59418500	-2.46225500	H	2.99161600	-3.89419200	1.11598400
H	5.04883400	3.89473000	-1.66118900	H	3.69253900	-5.11904300	0.04825400
H	4.04948200	3.23378100	1.21699200	H	3.74732900	-3.31963300	-2.49754800
H	5.69094000	3.71032100	0.74487600	H	5.00323500	-4.45543300	-1.97028400
H	5.42454600	2.21715100	1.65780200	H	5.40992000	-2.76232600	-2.28975800
N	-2.85724700	-0.72151700	-0.73596200	N	-2.14620300	1.95537900	-0.01081900
N	-0.29562500	-1.48783900	-0.12139400	N	0.60560900	1.95392900	-0.13279400
C	-3.39099200	-4.27399400	0.14389100	C	-1.43986800	5.58970400	-0.00487800
C	-2.12972700	-4.65170100	0.45625800	C	-0.08723700	5.58926000	-0.01009700
C	0.27277400	-4.09127600	0.67060900	C	2.04270600	4.33312000	-0.04646300
C	0.93419100	-1.85749000	0.16396300	C	1.92145100	1.95591200	-0.15173900
C	-5.17553000	-1.23811700	-1.04268700	C	-4.22701000	3.13850400	0.03401800
C	-4.96707600	-2.52595700	-0.63099800	C	-3.57449600	4.33841000	0.00847700
C	-4.07770600	-0.36186500	-1.05881300	C	-3.45975700	1.95839600	0.02176700
C	-1.04888700	-3.72671200	0.37176600	C	0.63990200	4.36470400	-0.03952700
C	-3.67244800	-2.94115400	-0.27634600	C	-2.17011900	4.36604300	-0.01079200
C	1.27290800	-3.16441000	0.56259400	C	2.69293700	3.13115500	-0.09097300
C	-1.27919300	-2.38966500	-0.03089600	C	-0.04108100	3.12376600	-0.06526300
C	-2.63372000	-1.98660500	-0.36179400	C	-1.49242400	3.12650900	-0.02674400
H	-6.14600400	-0.88115200	-1.36219700	H	-5.30447900	3.06242300	0.08625800
H	2.30501700	-3.40864700	0.77327400	H	3.77223100	3.06247200	-0.08979600
H	-5.78544900	-3.23721300	-0.58501500	H	-4.12525000	5.27346700	0.01534200
H	0.48795500	-5.10816500	0.98261500	H	2.59676400	5.26579500	-0.01932700
H	-4.21089400	-4.98223900	0.20345300	H	-1.99375500	6.52249900	0.01155200
H	-1.91842600	-5.66798000	0.77215300	H	0.46778800	6.52141400	0.00369100
Ligand 3-C3							
N	-3.29252800	2.28740700	0.34493700				
N	-4.43341300	1.64888200	0.30768700				
N	-2.13672100	0.34421100	-0.31815700				
C	-2.17887300	1.62397200	0.03667500				
C	-4.47744300	0.37082000	-0.04729300				
C	3.60052000	-1.53286600	-1.55302200				
C	-3.28782100	-0.29948800	-0.38616000				
C	-2.71782700	-2.57776400	0.36360200				
H	-2.64370100	-3.62930000	0.07394500				
H	-3.36376900	-2.51153400	1.24182200				
H	-1.72442500	-2.23082900	0.65126300				
C	-2.31086400	-1.91887200	-2.00534600				
H	-2.27911000	-2.97015500	-2.30335900				
H	-1.30120500	-1.58974500	-1.76025400				
H	-2.65481000	-1.33458100	-2.86269300				

C	-3.25272600	-1.75248300	-0.81364900
C	-5.71993000	-1.78466100	-0.20452300
C	-4.66114100	-2.21204100	-1.20301600
H	-6.69363600	-2.20043400	-0.48098100
H	-5.48417500	-2.19707900	0.78225600
H	-4.90345900	-1.81133200	-2.19322500
H	-4.65594000	-3.30106700	-1.30991000
O	4.13885100	-1.92361100	-2.57547300
N	2.87963200	-2.34189900	-0.73589600
C	2.55228400	-2.00367800	0.61003600
C	3.52602600	-2.05215900	1.59640800
C	1.25238800	-1.65327900	0.95443800
C	3.20241400	-1.75755500	2.91445500
H	4.54293000	-2.31702300	1.32882100
C	0.93789100	-1.36903800	2.26951300
H	0.50829700	-1.54654900	0.17516300
H	3.97645400	-1.79375900	3.67420600
H	-0.07677300	-1.07510400	2.51951900
C	1.54509400	-1.11202300	4.69694100
H	0.88113800	-1.87731300	5.10967600
H	1.02170100	-0.15570000	4.77512200
H	2.43228300	-1.06455600	5.33005900
C	1.90442500	-1.41916500	3.27462400
C	2.63156700	-3.71196700	-1.17038500
C	3.69801500	-4.69671900	-0.72631400
H	2.57183900	-3.69332200	-2.25910300
H	1.65401000	-4.00224300	-0.77638800
H	3.44896500	-5.70133900	-1.07671600
H	4.66765000	-4.42102100	-1.14443800
H	3.77914400	-4.73154800	0.36243000
C	-5.85318800	-0.26273900	-0.08955100
C	-6.63117400	0.08435700	1.17990200
C	-6.60267300	0.30991400	-1.29925600
H	-6.76418200	1.16173800	1.27616200
H	-6.11070500	-0.27529900	2.07137500
H	-7.61556300	-0.39046500	1.14772400
H	-6.66257200	1.39720900	-1.22346200
H	-7.61873400	-0.09247900	-1.33251300
H	-6.10833900	0.06560200	-2.24230400
N	2.56028800	0.52524800	-0.84726600
N	0.20247600	1.80620600	-0.23682500
C	3.76092500	3.98941600	-0.36246200
C	2.61288000	4.60872200	-0.00363300
C	0.17458100	4.51053200	0.40628400

C -0.91987500 2.41761000 0.07724700 C 4.90203600 0.59439500 -1.34886400 C 4.94581300 1.93188100 -1.06430200 C 3.67637900 -0.07262800 -1.19552400 C 1.38369300 3.89061600 0.05583600 C 3.77245600 2.59874000 -0.67424400 C -0.98229900 3.78281100 0.42116000 C 1.34112900 2.50995400 -0.25065000 C 2.58033700 1.84152900 -0.60462200 H 5.77148500 0.04468100 -1.68570700 H -1.93624800 4.22217300 0.67676700 H 5.87342200 2.48964400 -1.14242200 H 0.16931600 5.56669200 0.65559400 H 4.69363700 4.54093100 -0.41853800 H 2.60603600 5.66673600 0.23669900	
Am(L1)(NO$_3$)$_3$-*is1*	**Eu(L1)(NO$_3$)$_3$-*is1***
Am -0.03727100 -1.49952100 0.10980200 N 0.67798800 0.97993400 0.61567800 O -0.15950600 -2.94226900 2.07979200 O -0.82444200 -0.93116100 2.41719100 O -1.58968900 -3.26385700 -0.49446700 O -1.27697100 -1.78328900 -2.00985700 O 1.50110100 -0.60411200 -1.63513500 O 1.60005800 -2.72310700 -1.31626500 O 2.82773900 -1.80907800 -2.83986200 O -2.74515300 -3.33669700 -2.32037800 O -0.72258000 -2.31981500 4.06940000 N -1.90507200 -2.81728600 -1.64305500 N 2.00445800 -1.72445900 -1.96991500 N -0.57441800 -2.07661000 2.90620300 C 0.16368400 3.27400800 0.99162200 C 1.47889100 3.51218300 1.34321900 C -0.19704700 1.98139400 0.63366300 C 1.94808300 1.21092200 0.93269600 H -0.58788000 4.05134000 1.00220200 H 1.79472800 4.50325400 1.64656200 C 2.39140800 2.47099300 1.31257600 H 3.42474700 2.63228700 1.58464200 N -1.83365100 0.37407900 -0.02320100 N -3.05209500 0.00976200 -0.32642900 N -2.51573300 2.59061200 0.31808200 C -1.59199300 1.64138000 0.28541500 C -4.03090100 0.90025900 -0.32978000	Eu -0.18048300 -1.73081400 0.19908200 N 0.79930800 0.68858900 0.50431500 O 0.49122000 -1.83910300 2.54710500 O -1.43066000 -0.97178300 2.18145100 O -0.90498400 -3.94334300 0.76101400 O -2.24485700 -2.78512600 -0.44758300 O 0.43380600 -0.97839700 -2.04726400 O 0.77399900 -3.04963400 -1.61569400 O 1.49137700 -2.21104000 -3.47232300 O -2.76428300 -4.81293000 0.08776400 O -0.71628000 -1.17590200 4.21087600 N -2.00466100 -3.89097900 0.13077700 N 0.91943600 -2.08969600 -2.42355500 N -0.55883600 -1.32834100 3.03278000 C 0.40154400 2.89765700 1.29013900 C 1.73031400 3.00279300 1.65551600 C -0.02602000 1.70978600 0.70922000 C 2.09303100 0.81422000 0.78475200 H -0.30853300 3.69681200 1.45276400 H 2.09530100 3.90020200 2.14076900 C 2.60125500 1.95923300 1.38400700 H 3.64849900 2.03623200 1.63783600 N -1.72754300 0.33439900 -0.25557600 N -2.92344800 0.14773000 -0.74222800 N -2.27149600 2.52872700 0.37926500 C -1.42218700 1.52111800 0.26079900 C -3.82658400 1.11538600 -0.68488500

C	-3.75573000	2.24077000	0.02417000	C	-3.50405200	2.33761900	-0.06147500
C	-4.62079900	4.20889800	-1.16727600	C	-4.11636000	4.57672000	-0.87771800
H	-5.35021200	5.02234200	-1.14763000	H	-4.78873300	5.42792100	-0.74516000
H	-4.74926400	3.65845700	-2.10128700	H	-4.18496600	4.24689000	-1.91634300
H	-3.61946500	4.64385000	-1.16752300	H	-3.09374600	4.91373600	-0.69761900
C	-4.64830400	4.16690800	1.32537400	C	-4.41077000	4.01632400	1.53399300
H	-4.72399300	3.55730800	2.22906700	H	-4.61936400	3.23919000	2.27313300
H	-5.43824400	4.92109200	1.35911200	H	-5.15072100	4.81062000	1.65929500
H	-3.68428800	4.67540400	1.33619400	H	-3.42298700	4.42811200	1.74170400
C	-5.91063100	-0.47323600	0.47562800	C	-5.86402200	-0.22486200	-0.35065000
H	-6.88510300	-0.89783100	0.22248000	H	-6.83084700	-0.51052500	-0.77262800
H	-6.01828500	0.10488200	1.39637300	H	-6.03319500	0.17517300	0.65165200
H	-5.21917300	-1.29440600	0.67202800	H	-5.24837400	-1.12115000	-0.25571000
C	-5.32028100	-0.49107300	-1.94785500	C	-5.00629700	0.16042100	-2.65731300
H	-6.32541300	-0.82174500	-2.22151200	H	-5.98973500	-0.05116500	-3.08459100
H	-4.69913400	-1.37188300	-1.78926400	H	-4.44592200	-0.77227400	-2.59487500
H	-4.90620500	0.06625000	-2.79179200	H	-4.47920100	0.83408300	-3.33813100
C	-4.81640800	3.31608700	0.06659500	C	-4.49548500	3.46503200	0.11042400
C	-5.40410500	0.38159200	-0.69405900	C	-5.18003200	0.79192000	-1.27513200
C	-6.34449500	1.56217900	-0.95811500	C	-6.00595000	2.07640100	-1.39330300
C	-6.20707900	2.67316900	0.06473500	C	-5.91483500	2.95312300	-0.15842500
H	-7.37184600	1.18796500	-0.97497700	H	-7.04695400	1.80339300	-1.58754200
H	-6.14986300	1.95513300	-1.96154300	H	-5.67094100	2.63747300	-2.27242800
H	-6.41833400	2.28310300	1.06605400	H	-6.26158300	2.39398300	0.71682100
H	-6.94939100	3.45534400	-0.11904100	H	-6.58169800	3.81525500	-0.25173000
C	2.77534700	-0.04691800	0.99945500	C	2.86961800	-0.43642400	0.45906100
O	2.18069600	-1.09864700	1.25082100	O	2.24485900	-1.49587000	0.38993600
C	4.79301700	1.04287000	0.18829400	C	4.93040400	0.76349200	-0.06613800
C	5.85925700	1.69629400	0.79578800	C	6.02474800	1.15517600	0.69606500
C	4.42003100	1.38568300	-1.10496900	C	4.58154900	1.49675400	-1.19237300
C	6.53117800	2.69767400	0.11707900	C	6.74467500	2.28285000	0.34182900
H	6.15147300	1.43137000	1.80602600	H	6.29889400	0.58486200	1.57673800
C	5.09643600	2.39795700	-1.76772700	C	5.30432000	2.62984500	-1.53044100
H	3.60757800	0.85471900	-1.59124500	H	3.74536700	1.17574100	-1.80396200
H	7.35765800	3.20594900	0.60286900	H	7.59191800	2.58370500	0.94923000
C	6.16196900	3.06863900	-1.17523300	C	6.39758800	3.04241200	-0.77471000
H	4.79508100	2.65820800	-2.77688900	H	5.01802000	3.19664600	-2.41002100
C	6.91582600	4.13038800	-1.91549000	C	7.20110200	4.24389600	-1.16724200
H	6.28551600	4.62227200	-2.65788800	H	6.60498400	4.95041100	-1.74660600
H	7.77050800	3.69959900	-2.44621400	H	8.05623700	3.95264700	-1.78491700
H	7.30473400	4.89115400	-1.23618300	H	7.59503500	4.76348800	-0.29188500
C	4.87395800	-1.21774400	1.18978800	C	4.89236000	-1.69591800	0.11396900
C	5.07952100	-2.12619400	-0.00575700	C	4.94579900	-2.15561900	-1.32965500
H	5.83386400	-0.88453300	1.58891700	H	5.89885800	-1.56186900	0.51466500

H	4.33611600	-1.73826800	1.98130500	H	4.37076900	-2.42500600	0.73233000
H	5.72539100	-2.95866900	0.28128300	H	5.50304200	-3.09247400	-1.39163500
H	4.13429500	-2.54104200	-0.35588500	H	3.94554500	-2.33463400	-1.72551500
H	5.55846400	-1.59728400	-0.83212800	H	5.45056200	-1.42210000	-1.96217700
N	4.11018900	-0.00108200	0.87632200	N	4.20110300	-0.40831600	0.28282600
Am(L1)(NO$_3$)$_3$-*is2*				**Eu(L1)(NO$_3$)$_3$-*is2***			
Am	-0.30546700	-0.99154200	-0.37988900	Eu	0.33244100	-1.03523800	0.45401900
N	-0.16052400	1.65548200	-0.11925800	N	0.19660100	1.56798800	0.09993400
O	-0.89455400	-0.58217600	-2.75061900	O	0.89808900	-0.27988300	2.70853500
O	1.16099800	-0.24473400	-2.25345600	O	-1.19499900	-0.37874100	2.27547300
O	-0.52825400	-3.25847900	-1.23811800	O	0.52698600	-3.13593900	1.58680800
O	1.22762000	-2.87721800	-0.06678300	O	-1.12519400	-2.93517400	0.23533700
O	-0.74404400	-0.40653300	2.01432400	O	0.71364200	-0.66718600	-1.93644900
O	-1.80414900	-2.10295900	1.24506600	O	1.77721600	-2.30003700	-1.04623700
O	-2.27932300	-1.34465600	3.21085700	O	2.22852900	-1.70713200	-3.07336800
O	0.86530600	-4.86129400	-0.84379200	O	-0.81787400	-4.79907200	1.28397600
O	0.48554000	0.05458900	-4.28509300	O	-0.53572500	0.22869600	4.24204900
N	0.53365900	-3.71928300	-0.72165400	N	-0.48491900	-3.67595600	1.04584000
N	-1.63342600	-1.29289500	2.19804500	N	1.59776200	-1.57046100	-2.05957800
N	0.25598000	-0.24925900	-3.14906400	N	-0.28547400	-0.13280800	3.12712600
C	1.13087300	3.61083700	-0.52234200	C	-1.09239800	3.52674000	0.49133600
C	-0.02880500	4.32546800	-0.75480700	C	0.06873600	4.23745400	0.72876800
C	1.01753100	2.26262700	-0.20188600	C	-0.98071400	2.17708100	0.17629400
C	-1.28019700	2.35721700	-0.26284100	C	1.31841800	2.26592900	0.24469800
H	2.11165000	4.05973000	-0.59827500	H	-2.07204500	3.97918200	0.56122100
H	0.01988400	5.36858500	-1.04417200	H	0.02183900	5.28100900	1.01687600
C	-1.25891100	3.70168800	-0.60597400	C	1.29846100	3.61056300	0.58705800
H	-2.17711100	4.24596700	-0.77815300	H	2.21599300	4.15377800	0.76507800
N	1.97499300	0.14698100	0.37206000	N	-1.93058400	0.05106400	-0.36009500
N	2.98059700	-0.60544000	0.72671400	N	-2.93028600	-0.71284900	-0.70397000
N	3.39731400	1.99312100	0.07696100	N	-3.35823100	1.90276100	-0.12888900
C	2.20158900	1.42743100	0.09072300	C	-2.16269800	1.33751900	-0.11431000
C	4.20845300	-0.10919800	0.76091200	C	-4.15886900	-0.21925900	-0.76434600
C	4.43390200	1.22804600	0.37681600	C	-4.39023900	1.12783400	-0.42105100
C	5.94626100	2.81274300	1.49847400	C	-5.88963800	2.67596500	-1.60887700
H	6.91655700	3.31328100	1.45222200	H	-6.86069600	3.17683000	-1.59005900
H	5.87361700	2.29858700	2.45897100	H	-5.80477800	2.13269500	-2.55220100
H	5.16399400	3.57336500	1.46290500	H	-5.10825100	3.43802500	-1.58690900
C	5.96043500	2.63817300	-0.98881200	C	-5.93465900	2.57754900	0.88216100
H	5.81333600	1.99696600	-1.86114000	H	-5.79719900	1.96363500	1.77544600
H	6.96784700	3.05808400	-1.04267600	H	-6.94322300	2.99717300	0.91103800
H	5.24175200	3.45615500	-1.04200100	H	-5.21785900	3.39808700	0.91876100
C	5.47715500	-2.09620600	0.05366300	C	-5.43379200	-2.18414300	-0.00913600

H 6.23074800 -2.83182300 0.34584900	H -6.18241000 -2.93041800 -0.28674100
H 5.79768900 -1.63159100 -0.88158200	H -5.76627800 -1.69079100 0.90699100
H 4.53695500 -2.61798100 -0.13407000	H -4.49504300 -2.69747000 0.20691000
C 4.87646600 -1.80653000 2.45357300	C -4.80751100 -1.96931100 -2.41062900
H 5.67755200 -2.48315300 2.76160200	H -5.60468000 -2.65632200 -2.70556500
H 3.97205200 -2.39142800 2.28680500	H -3.90416100 -2.54731500 -2.21652600
H 4.68957500 -1.10791800 3.27348000	H -4.61270200 -1.29652700 -3.25004700
C 5.80982400 1.84868900 0.31192400	C -5.76733400 1.74877800 -0.39177500
C 5.29730700 -1.06983000 1.18090500	C -5.24236900 -1.19361500 -1.16619800
C 6.59344500 -0.29426800 1.43607200	C -6.53634700 -0.42800100 -1.45953700
C 6.87630100 0.74981500 0.37211900	C -6.83238900 0.64767100 -0.43133100
H 7.41960600 -1.00837300 1.49459300	H -7.36107600 -1.14469400 -1.50551900
H 6.53662200 0.18424200 2.41978100	H -6.46881700 0.02023600 -2.45673600
H 6.94391900 0.26768900 -0.60868900	H -6.91149600 0.19559800 0.56282100
H 7.84836100 1.22010000 0.54699600	H -7.80254100 1.11154700 -0.63208800
C -2.50831200 1.49703800 -0.10965400	C 2.54117000 1.39837100 0.08270400
O -2.41392900 0.32109700 -0.46423600	O 2.43305100 0.21446900 0.40208600
C -4.77740000 1.09656300 0.44663200	C 4.80594000 0.97978200 -0.47129100
C -4.98559400 0.31445100 1.57287400	C 4.97746500 0.18873700 -1.59774900
C -5.65250200 1.02772800 -0.62320000	C 5.70182300 0.90090700 0.58025700
C -6.07726300 -0.53376500 1.62104400	C 6.05336400 -0.67763900 -1.66511400
H -4.28116600 0.34231100 2.39719700	H 4.25507500 0.22449200 -2.40600300
C -6.74439700 0.17566100 -0.56065400	C 6.77871800 0.03109300 0.49822400
H -5.47259900 1.62874300 -1.50711700	H 5.54922800 1.50670000 1.46602100
H -6.22273000 -1.15643000 2.49721700	H 6.16939400 -1.30755600 -2.54049100
C -6.97415000 -0.61873400 0.55777000	C 6.97168700 -0.77182700 -0.62077500
H -7.42545100 0.12226100 -1.40325300	H 7.47624400 -0.03013000 1.32668700
C -8.13207600 -1.56765900 0.60971900	C 8.11324800 -1.73902700 -0.69363200
H -8.86730000 -1.34303200 -0.16412800	H 8.85592000 -1.53882700 0.07974400
H -8.63295000 -1.53104600 1.57951400	H 8.61008900 -1.69494800 -1.66530700
H -7.79377300 -2.59694900 0.45849000	H 7.75862500 -2.76485800 -0.55756300
C -3.78421000 3.23043800 1.15399400	C 3.85187000 3.14736100 -1.12655900
C -4.71399700 4.23600200 0.50473600	C 4.77594400 4.13101900 -0.43659200
H -4.17175700 2.95545200 2.13924000	H 4.25727000 2.89207900 -2.10996900
H -2.79340600 3.65084600 1.31903300	H 2.86787300 3.57965800 -1.30160700
H -4.79979500 5.12237800 1.13659700	H 4.87697200 5.03267700 -1.04418500
H -4.35447600 4.54969200 -0.47828200	H 4.40188300 4.42135500 0.54816800
H -5.71270300 3.81553800 0.37622800	H 5.77019900 3.70191000 -0.30257300
N -3.64990200 1.98824300 0.39481300	N 3.69310000 1.88854400 -0.40038700
Am(L2)(NO$_3$)$_3$-*is1*	**Eu(L2)(NO$_3$)$_3$-*is1***
Am -0.00886000 -0.52952000 0.39794500	Eu -0.01633900 -0.52834500 0.42406100
N 0.59872100 2.08083100 0.27003300	N 0.60373300 2.04443400 0.26342000
N -1.96141500 1.25148400 0.55165500	N -1.94628200 1.23011500 0.55455700

O	-1.66523000	-0.78049800	-1.53416600	O	-1.66239800	-0.81094900	-1.49898400
O	0.04853700	0.41376200	-1.98356800	O	0.06901800	0.35771100	-1.93800600
O	0.68969900	-2.75625900	1.19415300	O	0.66444700	-2.67828400	1.31393800
O	0.69705800	-2.48867600	-0.93102300	O	0.64617300	-2.50936600	-0.81850000
O	1.56448800	-0.09039600	2.30784500	O	1.56974300	-0.02070500	2.29729200
O	-0.48672600	0.32469200	2.73611800	O	-0.49475100	0.30059300	2.73325300
O	1.01610300	0.69448200	4.24417600	O	0.99432200	0.73074700	4.23862500
O	1.49496600	-4.30575500	-0.07879000	O	1.43160900	-4.29676100	0.10513100
O	-1.53812900	0.22850700	-3.43807400	O	-1.49206000	0.16183400	-3.41843900
N	0.97937300	-3.22876100	0.05469600	N	0.93295400	-3.20805500	0.19508400
N	0.70952200	0.32156300	3.14366000	N	0.70211900	0.34874900	3.13658100
N	-1.06251200	-0.03897900	-2.36220600	N	-1.04025900	-0.09112600	-2.32861400
C	-3.97338100	2.91051200	1.42147400	C	-3.97134800	2.90021200	1.36826800
C	-3.17537400	0.76557400	0.78588500	C	-3.16083700	0.74462600	0.78632800
C	2.21121700	3.77910200	-0.19468800	C	2.23469700	3.72542700	-0.19740200
C	1.24075600	4.75022600	-0.04495200	C	1.27363800	4.70659800	-0.05296100
C	-3.24840800	-0.73750200	0.71442200	C	-3.22276900	-0.75984100	0.74004300
C	1.84132100	2.44887900	-0.04004600	C	1.85135600	2.39905200	-0.04157300
C	-4.22231400	1.56434800	1.22128900	C	-4.21407100	1.54903600	1.19550300
C	-1.71879800	2.54980700	0.71261300	C	-1.70889600	2.53182900	0.69117800
C	-0.34284200	3.01501900	0.41034900	C	-0.32889800	2.98834500	0.39651500
H	3.23695900	4.01845500	-0.43726600	H	3.26383900	3.95401300	-0.43592300
H	-5.19779500	1.14057000	1.41455000	H	-5.19009900	1.12677800	1.38900900
H	1.48628000	5.79791300	-0.17214700	H	1.53065700	5.75159200	-0.17963900
H	-4.75668900	3.56213000	1.79003400	H	-4.76068700	3.55699000	1.71410800
O	-2.25861000	-1.37435800	1.08233200	O	-2.22242200	-1.38066900	1.10482700
N	-4.37828100	-1.35080100	0.33512600	N	-4.35119800	-1.39058600	0.38480900
C	-5.39355600	-0.70403900	-0.42683100	C	-5.37955300	-0.76939000	-0.38035600
C	-6.71581100	-0.74274200	-0.00158900	C	-6.69871700	-0.81476900	0.05830100
C	-5.07211000	-0.08978800	-1.63077600	C	-5.07572400	-0.17187100	-1.59565100
C	-7.70372300	-0.14650400	-0.76722000	C	-7.69894400	-0.24254500	-0.70701800
H	-6.96863000	-1.23660300	0.93019100	H	-6.93664500	-1.29382600	1.00167200
C	-6.07038100	0.51269800	-2.37949500	C	-6.08833600	0.40843600	-2.34538100
H	-4.04699300	-0.11252200	-1.98654100	H	-4.05303000	-0.18680900	-1.95886900
H	-8.73378800	-0.18429800	-0.42808000	H	-8.72524900	-0.28383200	-0.35642300
H	-5.80809300	0.98422400	-3.32082400	H	-5.83956400	0.87012000	-3.29504500
C	-8.46731900	1.16967600	-2.77255400	C	-8.50222100	1.01621900	-2.73038900
H	-8.23582800	1.13778000	-3.83857200	H	-8.14183400	1.31233600	-3.71622300
H	-8.56696900	2.22306800	-2.49231400	H	-8.89457100	1.90996800	-2.23612800
H	-9.43911300	0.69745000	-2.61900700	H	-9.34088200	0.32935900	-2.86756000
C	-7.39876600	0.50034000	-1.96325500	C	-7.41157200	0.38706800	-1.91835100
C	-4.40426700	-2.81938300	0.41835400	C	-4.36043200	-2.85778500	0.49360200
C	-4.61548800	-3.33158800	1.82910000	C	-4.54078700	-3.34771600	1.91645300
H	-3.45734000	-3.18797500	0.01814700	H	-3.41736500	-3.22393000	0.08200700

H	-5.20310400	-3.15084200	-0.24457100	H	-5.16788500	-3.20846800	-0.14870300
H	-4.61395200	-4.42358100	1.82446700	H	-4.52928000	-4.43958000	1.93013000
H	-3.81342100	-2.99773400	2.48786300	H	-3.72990200	-2.99552500	2.55448700
H	-5.57122000	-2.99649000	2.23855300	H	-5.49194700	-3.01413000	2.33765600
C	-2.71362100	3.41497800	1.16180800	C	-2.71085800	3.40369300	1.11006900
C	-0.05370600	4.36815900	0.25146900	C	-0.02610900	4.33827000	0.23802700
H	-2.50365900	4.46068600	1.33836900	H	-2.50677600	4.45411600	1.26397800
H	-0.83180700	5.11370500	0.33743400	H	-0.79660200	5.09193300	0.32155400
N	3.25537400	-0.84948000	-0.42434000	N	3.23418800	-0.91370900	-0.40032100
N	2.40628300	0.12507400	-0.24575900	N	2.39357300	0.06942800	-0.23389800
C	4.54004800	-0.58897600	-0.60816500	C	4.52272800	-0.66694300	-0.57859100
C	5.44044200	-1.78833600	-0.79991200	C	5.41327600	-1.87644500	-0.75184600
C	6.80684500	-1.32306800	-1.31347400	C	6.78491400	-1.42957800	-1.26761200
C	7.33037100	-0.10024300	-0.58447700	C	7.31813700	-0.20355700	-0.55105300
C	6.43972300	1.13355800	-0.76559200	C	6.43885400	1.03619100	-0.74657100
C	4.98924100	0.74784100	-0.58441100	C	4.98435200	0.66531500	-0.56543300
N	4.11143700	1.72083600	-0.41393100	N	4.11507800	1.64786900	-0.40583500
C	2.84280800	1.37762600	-0.24419400	C	2.84296700	1.31749100	-0.23779500
H	6.73167100	-1.11213100	-2.38558400	H	6.71368900	-1.22983200	-2.34215400
H	7.51356200	-2.15219700	-1.21748900	H	7.48393300	-2.26395300	-1.16096300
H	8.33882800	0.14737300	-0.92901400	H	8.32925500	0.03129600	-0.89676500
H	7.41927700	-0.31818800	0.48503100	H	7.40369800	-0.41082400	0.52082600
C	6.59272300	1.71974600	-2.17600500	C	6.60068800	1.60693500	-2.16228000
H	6.34899400	0.99362200	-2.95403200	H	6.35288900	0.87508600	-2.93365000
H	5.93523600	2.58199000	-2.30320400	H	5.95078300	2.47332000	-2.29994800
H	7.62453400	2.04742900	-2.32578600	H	7.63560100	1.92449200	-2.31257200
C	6.82859400	2.19889200	0.25915700	C	6.83486000	2.10803100	0.26857100
H	6.24009600	3.10735100	0.13059000	H	6.25515300	3.02054100	0.12923400
H	6.68108700	1.83860900	1.28012100	H	6.68097500	1.75942000	1.29263500
H	7.88533600	2.44945800	0.13740800	H	7.89424000	2.34758700	0.14742900
C	4.81658000	-2.75542600	-1.80794500	C	4.78419500	-2.85208400	-1.74817500
H	3.85872400	-3.13917200	-1.45713000	H	3.82159300	-3.22129700	-1.39475100
H	4.65608200	-2.26969900	-2.77396800	H	4.63136700	-2.37877500	-2.72157800
H	5.49360800	-3.59975300	-1.96158800	H	5.45372900	-3.70486300	-1.88735300
C	5.57270600	-2.49953500	0.55379000	C	5.53556000	-2.57025300	0.61183400
H	6.03176200	-1.86290600	1.31370100	H	5.99712400	-1.92696600	1.36454600
H	4.59060400	-2.80466000	0.91903900	H	4.54981300	-2.86235800	0.97801500
H	6.18962500	-3.39410400	0.43746900	H	6.14564000	-3.47128700	0.50998800
Am(L2)(NO$_3$)$_3$-*is2*				**Eu(L2)(NO$_3$)$_3$-*is2***			
Am	-0.26451600	0.00143300	-0.29725200	Eu	-0.28278700	0.05780900	-0.33491500
N	1.05123800	2.31753300	0.10213700	N	1.01153500	2.32276700	0.11271700
N	-1.64988500	2.24482200	0.02744700	N	-1.66169900	2.24927000	0.03123300
O	-0.66588200	1.36677000	-2.39934600	O	-0.82871500	1.15051000	-2.47748900

O	1.18226900	0.29834300	-2.33004000	O	1.25009500	0.69835700	-2.29330000
O	0.02118100	-2.23201200	0.72083000	O	-0.36186000	-2.25379600	0.41169600
O	-0.23852500	-2.19915100	-1.40430500	O	0.07081100	-1.93968900	-1.65917700
O	0.26811900	0.49376200	2.15159200	O	0.35568600	0.29869300	2.06345300
O	-1.74386900	-0.12716800	1.78921900	O	-1.73455400	-0.06375500	1.82901200
O	-1.11685200	0.34072600	3.80183600	O	-0.91101000	0.19072000	3.80910500
O	0.22285800	-4.06112400	-0.40964200	O	0.15395700	-3.93738700	-0.84024500
O	0.74094900	1.55846000	-4.02816900	O	0.53019200	1.70324900	-4.06437600
N	0.00776200	-2.87974300	-0.36558800	N	-0.04052400	-2.76055700	-0.70262500
N	-0.86932800	0.23713800	2.62779100	N	-0.77165200	0.14101200	2.61351400
N	0.43004000	1.09089000	-2.96547100	N	0.33070700	1.19972700	-2.98971700
C	-3.17020600	4.46495400	-0.53698400	C	-3.22707100	4.46579400	-0.39577700
C	-2.96038400	2.12913800	-0.15260200	C	-2.97725900	2.12067200	-0.10000000
C	3.08780200	3.43780200	0.64710100	C	3.07835000	3.43296600	0.54247500
C	2.41391100	4.64062400	0.72569300	C	2.42133200	4.64621500	0.60507500
C	-3.43101300	0.69738600	-0.20062300	C	-3.42696800	0.68241700	-0.15654000
C	2.36180200	2.29305300	0.34024400	C	2.33021800	2.28756800	0.29775700
C	-3.76760900	3.21942200	-0.43857700	C	-3.80591900	3.20953500	-0.32160500
C	-1.06933300	3.43895300	-0.04001800	C	-1.09836100	3.45267200	-0.00583900
C	0.39598000	3.47613600	0.18559000	C	0.37317300	3.49127900	0.17666300
H	4.15066400	3.35751100	0.82649500	H	4.14631400	3.34606700	0.68443200
H	-4.82758500	3.09115500	-0.61330400	H	-4.86959900	3.07475800	-0.46462100
H	2.94312200	5.55262500	0.97524300	H	2.97047100	5.55925200	0.80224300
H	-3.76127100	5.33714900	-0.79014300	H	-3.83752200	5.33821800	-0.59672400
O	-2.71374500	-0.09917200	-0.80712700	O	-2.69311400	-0.09958800	-0.76008300
N	-4.59533200	0.34050000	0.35696800	N	-4.58851100	0.30257200	0.39265800
C	-4.98892200	-1.03619500	0.23120300	C	-4.95656100	-1.08015900	0.25106900
C	-5.85966300	-1.41894700	-0.77330400	C	-5.86820700	-1.45718600	-0.71857500
C	-4.49811800	-1.97340200	1.12927000	C	-4.39782300	-2.02840600	1.09656000
C	-6.24696800	-2.74704300	-0.87549500	C	-6.23050500	-2.79135100	-0.83677700
H	-6.22428900	-0.68255200	-1.48027100	H	-6.28328700	-0.71227600	-1.38779000
C	-4.89145900	-3.29452500	1.01442300	C	-4.76540000	-3.35498300	0.96479300
H	-3.78660500	-1.66653300	1.88801600	H	-3.65445200	-1.72434400	1.82519300
H	-6.92694900	-3.04366100	-1.66705000	H	-6.94282600	-3.08367300	-1.60100600
H	-4.49398000	-4.02680800	1.70939600	H	-4.31292500	-4.09557700	1.61587200
C	-6.16020200	-5.14543400	-0.11663600	C	-6.05275300	-5.20530300	-0.14536500
H	-6.44703100	-5.56741700	0.84930600	H	-6.34774700	-5.63732500	0.81399200
H	-5.32326800	-5.74031200	-0.49381700	H	-5.20196100	-5.78592400	-0.51304500
H	-6.99595900	-5.27221500	-0.80616000	H	-6.87718900	-5.33968200	-0.84688800
C	-5.77004500	-3.70463800	0.01257100	C	-5.68637900	-3.75966400	-0.00088500
C	-5.28272600	1.11361000	1.39038800	C	-5.28335800	1.04606800	1.44315900
C	-6.72004400	1.44117800	1.04128100	C	-6.72503500	1.36663800	1.10583200
H	-4.70855500	2.01819700	1.58568800	H	-4.71792100	1.95131400	1.65943000
H	-5.24575000	0.52102800	2.30933300	H	-5.23806500	0.43259700	2.34796000

H -7.18511200 1.98464400 1.86634900	H -7.19125700 1.89048500 1.94291200
H -6.78834400 2.06045800 0.14352400	H -6.80386800 2.00136600 0.21973600
H -7.29876700 0.53232700 0.86834700	H -7.29629000 0.45587400 0.91912600
C -1.80935100 4.58315900 -0.33035700	C -1.86235000 4.59679400 -0.22640400
C 1.05019700 4.66375400 0.50114200	C 1.05105000 4.68104400 0.42621200
H -1.32707200 5.54555900 -0.43263500	H -1.39878000 5.57073200 -0.30049100
H 0.49934900 5.58971000 0.59347500	H 0.51760200 5.61876900 0.49806200
N 2.84931900 -1.26565200 -0.00156400	N 2.77805900 -1.28169500 -0.00032500
N 2.28450300 -0.09519900 0.11333600	N 2.22924200 -0.10178200 0.07614800
C 4.16474900 -1.38266100 0.08839000	C 4.09146400 -1.41358100 0.10830500
C 4.72081000 -2.77864700 -0.07714100	C 4.63129100 -2.82032800 -0.01679100
C 6.24368500 -2.70591600 -0.22906300	C 6.15646900 -2.77181500 -0.15626100
C 6.89183200 -1.74427600 0.74875000	C 6.80956800 -1.79054600 0.79817100
C 6.44604200 -0.29253600 0.54447600	C 6.38349100 -0.34015500 0.54811800
C 4.94694100 -0.24038300 0.35714200	C 4.88531900 -0.27490500 0.35608300
N 4.35948300 0.94120200 0.42938400	N 4.31102600 0.91424200 0.40782500
C 3.04265800 0.97936800 0.28686500	C 2.99650800 0.96599900 0.25209000
H 6.48617200 -2.41067700 -1.25545100	H 6.41160500 -2.51012300 -1.18855100
H 6.65311300 -3.71168000 -0.09912700	H 6.55106900 -3.77874900 0.00647000
H 7.98159700 -1.78730500 0.66216300	H 7.89929900 -1.84978300 0.72095000
H 6.65596000 -2.04670800 1.77465400	H 6.56265800 -2.05949900 1.83084800
C 7.09523800 0.31133500 -0.70841700	C 7.04188000 0.21610600 -0.72191900
H 6.86063300 -0.25765400 -1.61007600	H 6.79963100 -0.37612300 -1.60640400
H 6.75012700 1.33588900 -0.85929500	H 6.71133800 1.24042100 -0.90410500
H 8.18120800 0.32616200 -0.58634100	H 8.12792800 0.21945800 -0.59944300
C 6.84664600 0.54183800 1.76112000	C 6.79414100 0.52559800 1.73902000
H 6.57726300 1.58989600 1.62894700	H 6.53976300 1.57275800 1.57451600
H 6.36259300 0.17565600 2.66986300	H 6.30361300 0.19450600 2.65769700
H 7.92813900 0.47766100 1.90440700	H 7.87443400 0.45048800 1.88604500
C 4.11354100 -3.43754700 -1.31741200	C 4.02823700 -3.50216100 -1.24687400
H 3.03497900 -3.55806000 -1.21863400	H 2.94666400 -3.60455300 -1.16141200
H 4.31134400 -2.84865900 -2.21657900	H 4.24583200 -2.93899200 -2.15784900
H 4.55981500 -4.42610700 -1.45330600	H 4.46248700 -4.49979700 -1.35255200
C 4.32642700 -3.59560800 1.16073200	C 4.21668100 -3.60108900 1.23744000
H 4.75245000 -3.18616900 2.07984600	H 4.64143000 -3.17510100 2.14958000
H 3.24058400 -3.61546200 1.26989900	H 3.13005200 -3.60301400 1.33899400
H 4.68051500 -4.62336300 1.04777600	H 4.55652300 -4.63629400 1.15247100
Am(L3)$(NO_3)_3$-*is1*	**Eu(L3)$(NO_3)_3$-*is1***
Am -0.04392500 -0.60438700 0.52666400	Eu -0.04674400 -0.60656800 0.58750300
O 0.38209400 0.57859800 2.72659300	O 0.47739900 0.14599300 2.86942400
O -1.65207500 0.05289000 2.33966300	O -1.56574200 0.47736500 2.34549000
O -0.77463600 -2.69456100 -0.57049800	O -0.42156800 -2.88186700 -0.16716800
O -0.71890700 -2.73196800 1.57041600	O -1.16539000 -2.39807600 1.77908000

O	-0.05029100	-0.00697300	-1.96482900	O	-0.30569100	-0.26955900	-1.88004000
O	1.64167700	-1.14465000	-1.32529500	O	1.60213900	-1.07746800	-1.36913800
O	1.53349100	-0.44953600	-3.36602600	O	1.16051800	-0.60768100	-3.42995000
O	-1.52630600	-4.42001400	0.48931400	O	-1.60045700	-4.33166400	0.91861500
O	-1.14921500	1.10748200	4.15671700	O	-0.85918900	1.05758500	4.30230800
N	-1.02543200	-3.32830100	0.49528900	N	-1.08301000	-3.25118400	0.84847900
N	1.05207500	-0.53334700	-2.26320200	N	0.83148800	-0.65424100	-2.27087600
N	-0.81840800	0.59775500	3.12007900	N	-0.66292500	0.57771200	3.21691300
C	3.21188100	-0.78800200	0.91941800	C	3.18869900	-0.86127600	0.89042100
O	2.20552300	-1.34293100	1.36496200	O	2.16930100	-1.41706800	1.29944200
N	4.34708600	-1.46298400	0.68150300	N	4.31720400	-1.54610200	0.64604600
C	5.37201900	-0.97866700	-0.18154100	C	5.35004500	-1.05984200	-0.20559000
C	5.06760100	-0.59552500	-1.48133100	C	5.04995700	-0.64026200	-1.49525900
C	6.68810100	-0.92993500	0.26364300	C	6.66744300	-1.04504800	0.23785300
C	6.07637700	-0.13462000	-2.31336000	C	6.06527800	-0.17833300	-2.31865600
H	4.04547600	-0.67458400	-1.83807500	H	4.02425200	-0.69035100	-1.84784500
C	7.68561600	-0.47773300	-0.58223100	C	7.67129700	-0.59105800	-0.59960500
H	6.92546100	-1.23116700	1.27824500	H	6.90077400	-1.37438300	1.24459800
H	5.82574800	0.16572100	-3.32533200	H	5.81930500	0.15041600	-3.32295700
H	8.70877400	-0.43597700	-0.22301800	H	8.69571000	-0.57596600	-0.24188800
C	8.48839500	0.39061700	-2.80330500	C	8.48578100	0.31342200	-2.80185400
H	8.94809400	-0.46018100	-3.31580200	H	8.92855100	-0.53381100	-3.33478500
H	9.28005400	0.90709800	-2.25711500	H	9.28800100	0.80226300	-2.24576900
H	8.10424300	1.06463900	-3.57045200	H	8.11297300	1.01194200	-3.55252300
C	7.39826500	-0.06891400	-1.88410800	C	7.38901900	-0.14691200	-1.89097600
C	4.37230000	-2.89351400	1.01365600	C	4.31080200	-2.98650800	0.93707300
C	3.91053600	-3.76904600	-0.13501700	C	3.78102500	-3.81682900	-0.21594600
H	3.73302800	-3.03086200	1.88457500	H	3.70072900	-3.13067300	1.82794300
H	5.39900200	-3.13363300	1.29778600	H	5.33994800	-3.26190200	1.17613400
H	3.93677400	-4.81676700	0.17141700	H	3.80385100	-4.87405800	0.05664400
H	2.89038100	-3.51995000	-0.42880700	H	2.75207100	-3.54386700	-0.45261000
H	4.55812900	-3.65385600	-1.00667800	H	4.39114000	-3.68470300	-1.11200500
N	-3.32751700	-0.95035700	-0.30031100	N	-3.30190900	-0.99468000	-0.23384000
N	-2.45627200	0.01765400	-0.24208100	N	-2.43902400	-0.02192500	-0.15706600
C	-4.60292300	-0.68740900	-0.54472300	C	-4.57123700	-0.73924200	-0.51810600
C	-5.53220400	-1.87935300	-0.57627000	C	-5.49508100	-1.93515400	-0.56457700
C	-6.98507700	-1.39301800	-0.57619400	C	-6.94980000	-1.45573700	-0.60644700
C	-7.22028800	-0.22748900	-1.51806200	C	-7.16577600	-0.29535000	-1.55887900
C	-6.42664300	1.02455600	-1.13026400	C	-6.38735000	0.96148900	-1.15644300
C	-5.00583500	0.64182100	-0.78415800	C	-4.97186800	0.58648400	-0.78042400
N	-4.11545500	1.61392200	-0.68125300	N	-4.08489900	1.56197300	-0.67916700
C	-2.86798100	1.27146000	-0.39728500	C	-2.84422200	1.22697000	-0.35972000
H	-7.26562500	-1.10828900	0.44341700	H	-7.25917100	-1.16831300	0.40392600
H	-7.63169900	-2.23332700	-0.84424700	H	-7.58475800	-2.30052900	-0.88802300

H	-8.28282600	0.03141600	-1.54808100	H	-8.22831900	-0.04114800	-1.61676400
H	-6.94890300	-0.51744300	-2.53876700	H	-6.86728300	-0.58787600	-2.57130600
C	-7.04040600	1.70540900	0.10088700	C	-7.02931400	1.64062800	0.06123700
H	-7.08541900	1.03704800	0.96291400	H	-7.08653900	0.97406000	0.92390000
H	-6.45190500	2.57970100	0.38523200	H	-6.45203400	2.51935500	0.35496700
H	-8.05688300	2.03297500	-0.13132600	H	-8.04321300	1.96131900	-0.19109800
C	-6.42877000	2.01343100	-2.29604100	C	-6.37216100	1.94854400	-2.32346900
H	-5.90239400	2.93233300	-2.03723000	H	-5.85737600	2.87136300	-2.05576100
H	-5.95292400	1.58388500	-3.18109500	H	-5.87515200	1.52091000	-3.19772900
H	-7.45996700	2.26586800	-2.55525300	H	-7.39959300	2.19334800	-2.60411000
C	-5.28846300	-2.76369900	0.64827300	C	-5.28121300	-2.80756400	0.67425500
H	-4.28022000	-3.17718200	0.64855700	H	-4.26949100	-3.21049000	0.71405400
H	-5.42903800	-2.20404500	1.57636900	H	-5.45723000	-2.24114200	1.59213800
H	-6.00088800	-3.59269000	0.63988100	H	-5.98568300	-3.64309700	0.65046500
C	-5.21986900	-2.68961000	-1.84166300	C	-5.14832900	-2.75404200	-1.81514700
H	-5.40069800	-2.11762200	-2.75488600	H	-5.30947900	-2.19036400	-2.73714200
H	-4.17445200	-3.00331600	-1.83982400	H	-4.10192000	-3.06267700	-1.78645900
H	-5.84840500	-3.58329700	-1.86765400	H	-5.77134100	-3.65128700	-1.84897200
N	1.93179600	1.14158000	0.47568200	N	1.92910300	1.09107900	0.51212100
N	-0.62277600	1.96115800	0.04468700	N	-0.59300500	1.91752900	0.04411500
C	2.40524200	4.79879600	0.40849000	C	2.43908700	4.74171100	0.42671100
C	1.14426100	5.20598000	0.13133500	C	1.17838200	5.15715500	0.15596600
C	-1.23706000	4.64168000	-0.30739800	C	-1.21160700	4.60043900	-0.27979900
C	4.22575600	1.58443600	0.91949500	C	4.23408300	1.50454500	0.91733000
C	3.99949100	2.93363600	0.82561900	C	4.02266300	2.85767300	0.83468200
C	3.15050100	0.70686500	0.72173500	C	3.14662300	0.63886300	0.73224700
C	0.08275800	4.26465300	-0.01566100	C	0.10976800	4.22359200	0.00635500
C	2.71241300	3.41240600	0.54022700	C	2.73987000	3.35334100	0.55750500
C	-2.20474400	3.68280300	-0.44237300	C	-2.18005400	3.64058300	-0.40978800
C	0.34064600	2.88745800	0.13515400	C	0.36453200	2.84612100	0.14893400
C	1.69213700	2.45340600	0.38847900	C	1.71026400	2.40478800	0.41283400
H	5.21157700	1.20209200	1.14296700	H	5.21895500	1.11052800	1.12407200
H	-3.22988700	3.92792400	-0.68229800	H	-3.20761900	3.88738200	-0.63766100
H	4.81054800	3.63802400	0.97520400	H	4.84406800	3.55061400	0.98125800
H	-1.47775900	5.69205600	-0.43111400	H	-1.45501600	5.65076800	-0.39849300
H	3.20489100	5.52126500	0.52829300	H	3.24250100	5.46038900	0.54404200
H	0.91752900	6.26068600	0.02106800	H	0.95888000	6.21397800	0.05121000
C	-1.85293700	2.33744400	-0.25422400	C	-1.82783000	2.29351000	-0.23367800
Am(L3)(NO$_3$)$_3$-*is2*				**Eu(L3)(NO$_3$)$_3$-*is2***			
Am	0.25293100	-0.15810000	0.35164300	Eu	0.27218300	-0.13698000	0.33124700
O	0.93687900	0.55102600	2.62698400	O	0.83345100	0.88674500	2.49913300
O	-1.16854000	0.70634600	2.30301500	O	-1.25900600	0.51648700	2.28994400
O	0.22541500	-2.52463600	-0.37872100	O	0.36990600	-2.44775700	-0.41102100

O	-0.28298100	-2.17993200	1.67348000	O	-0.13162300	-2.13220300	1.64380100
O	-0.45236300	-0.04782200	-2.06145800	O	-0.36955800	0.08218800	-2.06647500
O	1.66003000	-0.27286500	-1.84599900	O	1.72425700	-0.25394000	-1.82523800
O	0.79234900	-0.17733400	-3.82164600	O	0.89969300	-0.03846700	-3.80975000
O	-0.49007000	-4.16068800	0.83694000	O	-0.18886200	-4.13053000	0.82373700
O	-0.34410800	1.23159500	4.22939100	O	-0.51430800	1.43556100	4.09702100
N	-0.19177900	-3.00238300	0.71702700	N	0.01077400	-2.95420800	0.69213900
N	0.67304700	-0.16887800	-2.62392500	N	0.75934800	-0.07164100	-2.61390000
N	-0.20103000	0.84259700	3.10173000	N	-0.32601000	0.96120400	3.00741300
C	3.45426900	0.53001300	0.09874300	C	3.44055300	0.50815800	0.14264400
O	2.73519100	-0.26628300	0.69847300	O	2.70668500	-0.26788500	0.75218300
N	4.61605400	0.16251300	-0.46451400	N	4.60805200	0.12237400	-0.39368700
C	4.99592000	-1.21741800	-0.32683800	C	4.97793300	-1.25641200	-0.22219600
C	5.91516500	-1.58883000	0.63762400	C	5.89807700	-1.61025100	0.74797700
C	4.44185900	-2.16872400	-1.17207200	C	4.41226500	-2.22476500	-1.04014400
C	6.28991800	-2.92007300	0.75059300	C	6.26232800	-2.94129700	0.89414400
H	6.32636300	-0.84186400	1.30691900	H	6.31796800	-0.84967700	1.39623100
C	4.82204600	-3.49221100	-1.04602100	C	4.78150700	-3.54766100	-0.88053200
H	3.69201000	-1.87008100	-1.89647100	H	3.66240700	-1.93845500	-1.76944700
H	7.00824800	-3.20793900	1.51086700	H	6.98144000	-3.21532200	1.65879900
H	4.37366300	-4.23514700	-1.69728300	H	4.32338900	-4.30354200	-1.50974800
C	6.13182800	-5.33357100	0.05286500	C	6.08169600	-5.37065100	0.25943800
H	6.42771600	-5.75958100	-0.90890800	H	6.39126900	-5.81703300	-0.68880300
H	5.28803600	-5.92368600	0.42153400	H	5.22867000	-5.94904200	0.62522100
H	6.95990300	-5.46226400	0.75114000	H	6.89764200	-5.48979800	0.97350600
C	5.75112900	-3.89104500	-0.08557400	C	5.71162700	-3.92911200	0.08605200
C	5.29236900	0.90321900	-1.52896400	C	5.29796200	0.83745300	-1.46692600
C	6.72960000	1.25439100	-1.20284700	C	6.73329700	1.19020200	-1.13469300
H	4.70957900	1.79340400	-1.76096500	H	4.72050900	1.72463500	-1.72270400
H	5.25626400	0.27407200	-2.42336600	H	5.26658200	0.19013700	-2.34841700
H	7.18400300	1.77422000	-2.04892200	H	7.19700200	1.69136900	-1.98696200
H	6.80156300	1.90164000	-0.32519200	H	6.79931100	1.85503300	-0.26977900
H	7.31652200	0.35585500	-1.00557300	H	7.31565200	0.29411200	-0.91408100
N	-2.89302800	-1.36202100	0.01383500	N	-2.83128600	-1.42207400	-0.05712700
N	-2.30920400	-0.19775500	-0.03559100	N	-2.26781700	-0.24805000	-0.08399900
C	-4.20446500	-1.45858900	-0.15004300	C	-4.14820900	-1.53274500	-0.16248300
C	-4.78479200	-2.85139700	-0.05511400	C	-4.70363600	-2.93751400	-0.09931200
C	-6.31315900	-2.76528900	0.01399900	C	-6.22685600	-2.87859600	0.05618000
C	-6.89675800	-1.76194600	-0.96213500	C	-6.87651000	-1.84587300	-0.84479300
C	-6.44727800	-0.32441000	-0.68101700	C	-6.43108700	-0.41402900	-0.53014100
C	-4.95803200	-0.29865600	-0.42298900	C	-4.93060000	-0.37541500	-0.34955000
N	-4.35153500	0.87597400	-0.44225600	N	-4.34227300	0.80891500	-0.35142900
C	-3.04272900	0.89079200	-0.23974100	C	-3.02639900	0.83589100	-0.20706300
H	-6.60968800	-2.50415800	1.03534500	H	-6.46998100	-2.66326200	1.10199300

H	-6.72438200	-3.76096900	-0.17448900	H	-6.63452100	-3.87219900	-0.15038500
H	-7.99005000	-1.79453100	-0.93663100	H	-7.96616300	-1.89637000	-0.76061600
H	-6.60786700	-2.02979200	-1.98414600	H	-6.64155000	-2.06818900	-1.89124400
C	-7.14820700	0.23904500	0.56270500	C	-7.07177500	0.08856100	0.77088300
H	-6.96045900	-0.36504900	1.45239300	H	-6.82978400	-0.54853400	1.62368100
H	-6.80194200	1.25391300	0.76745200	H	-6.72688300	1.09880800	0.99921300
H	-8.22725200	0.26993900	0.39189200	H	-8.15866700	0.11124300	0.65838400
C	-6.78211800	0.55996400	-1.88204800	C	-6.84154500	0.51215500	-1.67478200
H	-6.50712500	1.59878800	-1.69891500	H	-6.57167600	1.54703600	-1.46385800
H	-6.26046200	0.22165400	-2.78068900	H	-6.36390800	0.21857900	-2.61280900
H	-7.85649300	0.51448700	-2.07682600	H	-7.92403400	0.45760500	-1.81452600
C	-4.25643600	-3.55126500	1.19915800	C	-4.09819600	-3.68417200	1.09135000
H	-3.17503500	-3.68147600	1.16388200	H	-3.01867500	-3.79475100	0.99171300
H	-4.50330100	-2.98554200	2.10119800	H	-4.30109500	-3.16264700	2.03005700
H	-4.72033800	-4.53778200	1.28041500	H	-4.54344000	-4.68061100	1.15345000
C	-4.33178100	-3.63898900	-1.29181100	C	-4.30922200	-3.66220100	-1.39313000
H	-4.70321200	-3.20005400	-2.22094600	H	-4.73862400	-3.18967300	-2.27979200
H	-3.24205100	-3.66860000	-1.34308200	H	-3.22376700	-3.66938200	-1.50609100
H	-4.70124100	-4.66537900	-1.22601300	H	-4.65845700	-4.69700500	-1.35346900
N	1.67080300	2.06213100	-0.00965200	N	1.66562600	2.04039200	-0.01489600
N	-1.02281600	2.16452200	-0.14620700	N	-1.02166400	2.12954100	-0.09626200
C	1.15300700	5.71366200	-0.04040800	C	1.13485500	5.68823100	-0.03314600
C	-0.19590500	5.76601900	-0.15067000	C	-0.21546200	5.73444700	-0.13222400
C	-2.37924100	4.57817300	-0.31507900	C	-2.39591000	4.53170900	-0.26902500
C	3.80635000	3.09348900	0.13259600	C	3.79761700	3.07422200	0.14087400
C	3.22540300	4.33757400	0.12581000	C	3.21513300	4.31785900	0.12463900
C	2.98353400	1.96309400	0.03722500	C	2.97710100	1.94202300	0.04593600
C	-0.98018600	4.57495600	-0.20135000	C	-0.99568000	4.53983600	-0.17049300
C	1.83297100	4.46064500	0.01202900	C	1.82203600	4.43856000	0.01525900
C	-3.06087800	3.39100300	-0.34543600	C	-3.06886600	3.33888200	-0.29393400
C	-0.34711800	3.31911100	-0.13166200	C	-0.35425300	3.28893200	-0.10179000
C	1.09052200	3.26457000	-0.04041400	C	1.08359100	3.24103700	-0.03440200
H	4.87802700	2.98419700	0.22963300	H	4.86891100	2.96702000	0.24446900
H	-4.13748800	3.34802700	-0.43381000	H	-4.14557200	3.28781000	-0.37691100
H	3.83638700	5.23006200	0.20769100	H	3.82532900	5.21129100	0.20187400
H	-2.90956700	5.52240000	-0.37546600	H	-2.93453900	5.47143700	-0.32616400
H	1.73833300	6.62527500	0.00470400	H	1.71569200	6.60297900	0.00613500
H	-0.70614600	6.72180500	-0.19757100	H	-0.72983600	6.68808700	-0.17705300
C	-2.33829000	2.19127500	-0.24656000	C	-2.33778100	2.14442400	-0.19709700
$[Am(L3)_2NO_3]^{2+}$-*is1*				**$[Eu(L3)_2NO_3]^{2+}$-*is1***			
Am	0.00030000	-0.47952400	-0.00003900	Eu	-0.00016200	-0.49218000	0.00015600
N	-2.25509700	-1.45951200	0.88536100	N	2.24933600	-1.46536200	-0.87753700
N	-3.18757400	-1.78564100	0.01575600	N	3.17550300	-1.78640400	0.00090400

C	-4.22189900	-2.52223200	0.39795200	C	4.21381500	-2.52356600	-0.36835600
C	-4.33522500	-2.93356600	1.75281700	C	4.34037700	-2.94032200	-1.72019000
N	-3.40393600	-2.56100600	2.61694900	N	3.41644900	-2.57259800	-2.59405300
C	-2.38439100	-1.84919800	2.15099100	C	2.39120500	-1.86064200	-2.14037600
C	-5.19896100	-2.93048400	-0.68387200	C	5.17836000	-2.92944400	0.72547000
C	-6.50119900	-3.42977600	-0.04330900	C	6.48658700	-3.43422900	0.10179300
H	-7.08990900	-2.56863400	0.29477500	H	7.08205800	-2.57564100	-0.23083700
H	-7.10358500	-3.91758300	-0.81592700	H	7.07810200	-3.92240000	0.88255900
C	-6.26635400	-4.38451900	1.11486300	C	6.26313000	-4.39061800	-1.05738500
H	-5.72063500	-5.26815000	0.76589200	H	5.71180500	-5.27264600	-0.71313100
H	-7.22195400	-4.75757500	1.49559100	H	7.22238800	-4.76613200	-1.42634200
C	-5.49631000	-3.74515500	2.27867300	C	5.50756700	-3.75240000	-2.23129800
C	-4.52460200	-4.04448600	-1.50321700	C	4.49096600	-4.03864800	1.54067400
H	-4.29788200	-4.92803800	-0.90156100	H	4.27659300	-4.92664800	0.94098700
H	-3.58365000	-3.69073800	-1.93191100	H	3.54154000	-3.68326600	1.94894200
H	-5.18368300	-4.35395900	-2.31925000	H	5.13537500	-4.34156000	2.37074500
C	-5.50376200	-1.75018900	-1.60779300	C	5.47482000	-1.74643100	1.64842800
H	-6.23022500	-2.05909800	-2.36445800	H	6.19124200	-2.05389200	2.41518800
H	-4.60435400	-1.40072500	-2.11673500	H	4.56997800	-1.39299300	2.14469500
H	-5.93505000	-0.91025000	-1.05407600	H	5.91468300	-0.90962800	1.09670400
C	-6.39856800	-2.78099300	3.06956300	C	6.41924000	-2.78864000	-3.01188400
H	-6.81490900	-1.98702100	2.44386600	H	6.82739700	-1.99375800	-2.38195300
H	-5.84204200	-2.31248500	3.88490100	H	5.87263200	-2.32134800	-3.83460800
H	-7.23283900	-3.33747100	3.50461800	H	7.25913700	-3.34517500	-3.43591900
C	-4.98999400	-4.83859000	3.22313200	C	5.01320300	-4.84660200	-3.18104300
H	-5.83597900	-5.43799100	3.56934900	H	5.86353100	-5.44570400	-3.51699100
H	-4.49208200	-4.41689000	4.09728600	H	4.52526000	-4.42562400	-4.06113100
H	-4.28862500	-5.51035900	2.72034900	H	4.30640700	-5.51856100	-2.68615800
N	-0.30169500	-0.75535500	2.59690100	N	0.31303300	-0.77597000	-2.60279900
C	-1.30309800	-1.47345000	3.08669000	C	1.31724300	-1.49148700	-3.08673500
C	-1.34964500	-1.89820400	4.42387600	C	1.37214300	-1.91740900	-4.42363100
H	-2.19821500	-2.47917400	4.76105700	H	2.22331100	-2.49724500	-4.75649100
C	-0.30462400	-1.58292500	5.25601100	C	0.33142400	-1.60240400	-5.26201600
H	-0.30294400	-1.91307900	6.29020200	H	0.33644200	-1.93157100	-6.29651500
C	0.77394300	-0.82991700	4.76134900	C	-0.75055800	-0.85020900	-4.77290500
C	1.90042100	-0.46649800	5.56281800	C	-1.87340200	-0.48221700	-5.57784000
H	1.93203600	-0.80123200	6.59487000	H	-1.90179100	-0.81345500	-6.61114900
C	2.91058700	0.28142000	5.05269100	C	-2.88409600	0.26729300	-5.07013400
H	3.76151300	0.55293200	5.66910800	H	-3.73086000	0.54301100	-5.69043800
C	2.86675000	0.73935300	3.70024000	C	-2.84674300	0.72103100	-3.71572700
C	3.86608200	1.53852500	3.12442600	C	-3.84493500	1.52176000	-3.14020700
H	4.74601300	1.80175000	3.70327100	H	-4.72117700	1.79233500	-3.72128800
C	3.71959200	2.00642200	1.83928000	C	-3.70228200	1.98227200	-1.85145600
H	4.47680100	2.64342800	1.40478300	H	-4.45914000	2.61997700	-1.41758500

C	2.57508400	1.64398600	1.11083200	C	-2.56266300	1.61008800	-1.12000900
N	1.66898400	0.80767600	1.60389700	N	-1.65786300	0.77377400	-1.61401000
C	1.77754100	0.38640500	2.87325100	C	-1.76295400	0.36059200	-2.88519200
C	0.71470100	-0.42704000	3.40955400	C	-0.69833900	-0.45068500	-3.42003200
C	2.23442800	2.07657900	-0.29375700	C	-2.21530600	2.03136300	0.28636500
N	2.84073000	3.11730100	-0.88968700	N	-2.82281700	3.05860700	0.90191000
N	2.25519000	-1.46054100	-0.88496200	N	-2.24984900	-1.46487000	0.87757900
N	3.18763900	-1.78639400	-0.01525100	N	-3.17582500	-1.78604300	-0.00101600
C	4.22227400	-2.52262300	-0.39732900	C	-4.21440400	-2.52284200	0.36821200
C	4.33581600	-2.93401300	-1.75215100	C	-4.34142500	-2.93910600	1.72015700
N	3.40448000	-2.56179100	-2.61638600	N	-3.41766100	-2.57127800	2.59414900
C	2.38473000	-1.85018500	-2.15058600	C	-2.39215100	-1.85967400	2.14052000
C	5.19943800	-2.93038800	0.68459900	C	-5.17877300	-2.92885100	-0.72572200
C	6.50182300	-3.42945900	0.04416600	C	-6.48728000	-3.43310000	-0.10219900
H	7.10428600	-3.91703300	0.81687100	H	-7.07873600	-3.92136100	-0.88295200
H	7.09035300	-2.56823200	-0.29400200	H	-7.08260700	-2.57425000	0.23002000
C	6.26724900	-4.38440000	-1.11390800	C	-6.26434600	-4.38918000	1.05733400
H	7.22294700	-4.75732900	-1.49451700	H	-7.22378700	-4.76434000	1.42617300
H	5.72166800	-5.26808900	-0.76486800	H	-5.71315300	-5.27145200	0.71349400
C	5.49716700	-3.74532400	-2.27784800	C	-5.50891700	-3.75077500	2.23123000
C	5.50388700	-1.74978800	1.60825100	C	-5.47471500	-1.74606700	-1.64913900
H	5.93491100	-0.90984400	1.05433600	H	-5.91447900	-0.90896500	-1.09779200
H	6.23045800	-2.05830100	2.36497500	H	-6.19104500	-2.05359500	-2.41595900
H	4.60437800	-1.40048800	2.11712900	H	-4.56967000	-1.39303300	-2.14532200
C	4.52542400	-4.04439300	1.50422300	C	-4.49147200	-4.03849500	-1.54040200
H	3.58433900	-3.69084600	1.93279100	H	-3.54184400	-3.68350000	-1.94853800
H	5.18457400	-4.35341100	2.32037000	H	-5.13574800	-4.34148600	-2.37054700
H	4.29905900	-4.92819800	0.90280100	H	-4.27750700	-4.92637100	-0.94038700
C	4.99124800	-4.83894600	-3.22229500	C	-5.01500900	-4.84480000	3.18141900
H	5.83744300	-5.43807200	-3.56848000	H	-5.86554600	-5.44361300	3.51735300
H	4.49322100	-4.41743100	-4.09647300	H	-4.52717400	-4.42366400	4.06149100
H	4.29009200	-5.51094700	-2.71952500	H	-4.30825000	-5.51706700	2.68689800
C	6.39924100	-2.78097300	-3.06871900	C	-6.42056300	-2.78658600	3.01131700
H	6.81524100	-1.98678700	-2.44306700	H	-6.82841100	-1.99180900	2.38105200
H	5.84268400	-2.31274300	-3.88419600	H	-5.87404300	-2.31915900	3.83402300
H	7.23375000	-3.33724200	-3.50358600	H	-7.26067200	-3.34281500	3.43533000
N	0.30206900	-0.75643900	-2.59676900	N	-0.31388400	-0.77529600	2.60311700
C	1.30344800	-1.47467500	-3.08638500	C	-1.31835900	-1.49044300	3.08703900
C	1.34994500	-1.89986300	-4.42343600	C	-1.37364100	-1.91598400	4.42404100
H	2.19852600	-2.48090300	-4.76046800	H	-2.22501800	-2.49551800	4.75689100
C	0.30485900	-1.58490600	-5.25560100	C	-0.33300300	-1.60101700	5.26254400
H	0.30310500	-1.91540500	-6.28968100	H	-0.33831000	-1.92989800	6.29713200
C	-0.77371700	-0.83179400	-4.76110600	C	0.74928700	-0.84926800	4.77343000
C	-1.90027500	-0.46876200	-5.56263600	C	1.87210600	-0.48141700	5.57846600

H	-1.93192500	-0.80387300	-6.59456500	H	1.90020600	-0.81238400	6.61186900
C	-2.91047500	0.27923900	-5.05270500	C	2.88313900	0.26761300	5.07072900
H	-3.76148100	0.55043800	-5.66914900	H	3.72988900	0.54321500	5.69110400
C	-2.86657100	0.73766400	-3.70042600	C	2.84618000	0.72098700	3.71618800
C	-3.86594900	1.53691800	-3.12482800	C	3.84474500	1.52121000	3.14061900
H	-4.74595800	1.79982100	-3.70370200	H	4.72098600	1.79163600	3.72177200
C	-3.71945400	2.00531200	-1.83986200	C	3.70247000	1.98142900	1.85171900
H	-4.47682400	2.64230400	-1.40563200	H	4.45963300	2.61874700	1.41781700
C	-2.57483200	1.64333100	-1.11135500	C	2.56284500	1.60945300	1.12017500
C	-1.77726100	0.38515500	-2.87337700	C	1.76241000	0.36069500	2.88556300
C	-0.71440500	-0.42842500	-3.40946300	C	0.69743300	-0.45008700	3.42044100
C	-2.23404900	2.07648600	0.29305300	C	2.21581300	2.03052100	-0.28635000
N	-2.84092500	3.11686900	0.88901400	N	2.82391200	3.05725000	-0.90216900
O	-0.42619500	-2.75748400	-0.98275500	O	0.45968800	-2.72082200	0.96677600
N	-0.00138700	-3.44228500	0.00031400	N	0.00036700	-3.40595000	0.00073600
O	0.42502000	-2.75763000	0.98282900	O	-0.45946900	-2.72135800	-0.96544800
O	-0.00283800	-4.63917500	0.00086100	O	0.00082400	-4.60274000	0.00084800
N	-1.66865300	0.80697400	-1.60421300	N	1.65768100	0.77357300	1.61425500
O	-1.37391600	1.41893200	0.89773800	O	1.34217800	1.37382600	-0.87321800
C	-2.51757500	3.37856600	2.30207400	C	2.48253700	3.30816700	-2.31306700
C	-1.30653600	4.27845600	2.46639600	C	1.28153200	4.22294800	-2.46841200
H	-2.35497200	2.41573100	2.78560000	H	2.29909200	2.34257200	-2.78335400
H	-3.40264600	3.83921500	2.74482100	H	3.36709300	3.75175200	-2.77394500
H	-1.13172900	4.47741300	3.52645800	H	1.09188400	4.41152200	-3.52781000
H	-0.41355600	3.79852000	2.05879500	H	0.38880300	3.76066800	-2.04037700
H	-1.45479000	5.23952600	1.96761400	H	1.45115100	5.18785700	-1.98412700
O	1.37491900	1.41831800	-0.89856900	O	-1.34200300	1.37434800	0.87336300
C	2.93333700	4.94651800	0.73549900	C	-2.97059600	4.91575600	-0.68712100
C	4.90280400	4.37639300	-0.52662400	C	-4.91706000	4.27369600	0.57650000
C	3.64470800	5.95157000	1.37832900	C	-3.71030600	5.91593000	-1.30505100
H	1.88525000	4.78178400	0.96769600	H	-1.92078300	4.78008500	-0.93000900
C	5.59950100	5.38771200	0.11677600	C	-5.64246300	5.28016200	-0.04246900
H	5.39947400	3.75237900	-1.26374800	H	-5.39291600	3.62361100	1.30476000
H	3.14147200	6.56875800	2.11674900	H	-3.22731500	6.55935800	-2.03452500
H	6.64260200	5.55597200	-0.13464300	H	-6.68756400	5.41822400	0.21882000
C	5.74249600	7.30358300	1.74603100	C	-5.84235700	7.22382000	-1.63238900
H	5.78299100	8.18445100	1.09707800	H	-5.89542600	8.09214000	-0.96761600
H	6.77417300	7.01600700	1.96077000	H	-6.86960300	6.91740000	-1.84213400
H	5.27374400	7.60994700	2.68278000	H	-5.38982900	7.55675000	-2.56805100
C	4.98634000	6.19320300	1.08180700	C	-5.05537800	6.11907100	-0.99513100
C	2.51750800	3.37867600	-2.30282900	C	-2.48122800	3.30976600	2.31271100
C	1.30603000	4.27793100	-2.46742200	C	-1.27971000	4.22393300	2.46770600
H	2.35545800	2.41571200	-2.78628300	H	-2.29829100	2.34421400	2.78328100
H	3.40241000	3.83972300	-2.74549500	H	-3.36551200	3.75397900	2.77350800

H 1.13124900 4.47666400 -3.52752900	H -1.08989700 4.41272900 3.52703500
H 0.41324000 3.79758900 -2.05987100	H -0.38726000 3.76103300 2.03976000
H 1.45372200 5.23913500 -1.96873100	H -1.44882900 5.18878600 1.98313300
C 3.56630600 4.14573300 -0.20857200	C -3.57784400 4.08191400 0.24510200
C -3.56703600 4.14490100 0.20788500	C 3.57951400 4.08033200 -0.24566800
C -4.90360000 4.37491400 0.52596100	C 4.91887600 4.27112000 -0.57695500
C -5.60090100 5.38572400 -0.11766300	C 5.64485900 5.27737200 0.04173400
C -3.64644700 5.95034900 -1.37940500	C 3.71292300 5.91486100 1.30379100
C -2.93452600 4.94584100 -0.73641500	C 2.97266600 4.91493700 0.68616400
H -5.39990900 3.75078200 1.26322700	H 5.39442100 3.62043100 -1.30487900
H -6.64409100 5.55343400 0.13373500	H 6.69008700 5.41463400 -0.21945000
H -3.14359900 6.56763700 -2.11801300	H 3.23025900 6.55887300 2.03296900
H -1.88637300 4.78157600 -0.96865100	H 1.92274000 4.78000600 0.92898300
C -5.74469200 7.30144400 -1.74717000	C 5.84557600 7.22171300 1.63081800
H -5.28100100 7.60177600 -2.68840500	H 5.39633400 7.55117700 2.56930300
H -5.77734200 8.18546100 -1.10204100	H 5.89378600 8.09195900 0.96818000
H -6.77885000 7.01690400 -1.95367700	H 6.87437000 6.91701400 1.83529300
C -4.98823400 6.19132200 -1.08286100	C 5.05819100 6.11702500 0.99396000
$[Am(L3)_2NO_3]^{2+}$-*is2*	**$[Eu(L3)_2NO_3]^{2+}$-*is2***
Am -0.44995500 0.09423200 -0.18044800	Eu -0.47963500 0.00023500 -0.18338400
N -4.44742400 1.79622600 -1.19752700	N -4.67104200 1.01709200 -1.22541300
C -3.37697700 1.54586700 -0.43852400	C -3.58492000 0.93138800 -0.45363600
N -2.39826700 0.58594000 1.47521800	N -2.48029100 0.15776200 1.46506900
C -3.50312200 1.15410400 1.01336500	C -3.66228800 0.53060600 0.99945800
C -4.60367600 1.41422700 1.84569500	C -4.79503400 0.59604300 1.82764700
H -5.47891500 1.92125100 1.46389400	H -5.74373400 0.94571900 1.44463200
C -4.55673000 1.00317900 3.15690300	C -4.68144100 0.19703900 3.13922300
H -5.39849200 1.18736000 3.81717800	H -5.54446600 0.23342000 3.79672300
C -3.42146600 0.33621700 3.64378300	C -3.44983400 -0.26559100 3.62980900
C -3.31213700 -0.14906600 4.98316300	C -3.25700300 -0.72482600 4.96915900
H -4.15711400 -0.02693000 5.65322300	H -4.10921600 -0.75042800 5.64072100
C -2.17396000 -0.74862200 5.41262400	C -2.03138400 -1.11806900 5.39777000
H -2.09507600 -1.11378300 6.43167200	H -1.89037800 -1.46276400 6.41727600
C -1.04803400 -0.89599400 4.54473200	C -0.89641300 -1.07028200 4.52969600
C 0.16964700 -1.45609800 4.96633800	C 0.40114700 -1.40890800 4.94937200
H 0.26868800 -1.82868200 5.98130600	H 0.56610900 -1.75674900 5.96456500
C 1.23384900 -1.49807900 4.10016800	C 1.45469900 -1.26565500 4.08042300
H 2.20001400 -1.88591300 4.39536200	H 2.47458500 -1.47768900 4.37377300
C 1.06589200 -1.00373700 2.79724900	C 1.19973900 -0.81147700 2.77706500
N -0.09068400 -0.53004800 2.35146200	N -0.02222900 -0.54849800 2.33294700
C -1.12546700 -0.44698500 3.20717700	C -1.05250600 -0.64421000 3.19184800
C -2.34424200 0.16993500 2.74692900	C -2.35940200 -0.24517100 2.73417100
N 2.04225000 -0.31911800 0.71114000	N 2.02657600 0.03484300 0.68808900

C	2.22720300	-0.92007700	1.88530800	C	2.32347000	-0.52416200	1.85991400
N	3.39019200	-1.40117000	2.31193000	N	3.55609600	-0.78971400	2.27869600
C	4.44583000	-1.23816600	1.53114900	C	4.56057900	-0.44038000	1.49113500
C	4.28626600	-0.55107900	0.29895700	C	4.27275900	0.20747300	0.26125300
N	3.08455500	-0.12942200	-0.07250200	N	3.01267300	0.40798600	-0.10206400
C	5.43939300	-0.22460700	-0.62867800	C	5.34274400	0.73442900	-0.67362700
C	5.75697800	-1.83781100	1.98441200	C	5.96055000	-0.79629700	1.93520500
C	6.63835100	-1.12519400	-0.29854400	C	6.68473000	0.06059800	-0.35361800
H	6.46104500	-2.12388000	-0.71435300	H	6.68382100	-0.95385200	-0.76907300
H	7.51819300	-0.73816200	-0.82182500	H	7.47823200	0.59711300	-0.88300400
C	6.91958000	-1.22644800	1.19078600	C	6.99048900	0.01117500	1.13357000
H	7.81454200	-1.83162000	1.36419500	H	7.97981700	-0.42569400	1.29982000
H	7.14952200	-0.23506600	1.59763500	H	7.04410200	1.02779900	1.53954200
C	5.03641300	-0.43315900	-2.08957600	C	4.97216600	0.45901100	-2.13203700
H	4.71686300	-1.46345600	-2.27253300	H	4.84143800	-0.61167000	-2.31541700
H	5.89449000	-0.23108000	-2.73642100	H	5.77466900	0.81286300	-2.78495200
H	4.22334500	0.23310600	-2.38092700	H	4.05013700	0.96855800	-2.41500600
C	5.79437600	1.25657500	-0.41761400	C	5.43040300	2.25494600	-0.46188200
H	4.93447500	1.89117200	-0.65007400	H	4.46938000	2.72646400	-0.68615500
H	6.61574600	1.54035600	-1.08137200	H	6.18266400	2.68100500	-1.13143600
H	6.10383800	1.47133200	0.60861700	H	5.70506700	2.52051400	0.56237300
C	5.66213400	-3.35479200	1.73912800	C	6.13546800	-2.30625700	1.69036800
H	6.57974900	-3.83835400	2.08423500	H	7.12630100	-2.61875400	2.03030000
H	5.52933300	-3.60221300	0.68255500	H	6.04294100	-2.57437000	0.63452500
H	4.82418800	-3.78280200	2.29513500	H	5.38994600	-2.87577900	2.25104200
C	5.96801600	-1.59080600	3.47988900	C	6.13421900	-0.51415700	3.42925100
H	5.19166500	-2.06630900	4.08062400	H	5.45896100	-1.11974400	4.03504100
H	5.97584800	-0.52222400	3.71340800	H	5.95304200	0.53896400	3.66286000
H	6.93337900	-2.00417500	3.78298900	H	7.15980600	-0.74858800	3.72569300
N	0.26948100	-2.41194000	-0.50985000	N	0.69065900	-2.32382200	-0.51638300
N	-0.07809600	-3.30248800	0.39447600	N	0.53341400	-3.25505000	0.40002200
C	0.03069400	-4.59693500	0.12749100	C	0.86550900	-4.51128400	0.13528800
C	0.53770800	-5.01920700	-1.13040500	C	1.40820500	-4.84681200	-1.13341200
N	0.91895600	-4.10464600	-2.00929600	N	1.59690700	-3.88610200	-2.02527400
C	0.76098100	-2.82965800	-1.67501700	C	1.22039900	-2.65732200	-1.69202900
C	-0.45774300	-5.55032800	1.19712100	C	0.57924400	-5.52782900	1.21983700
C	0.06768700	-6.96316200	0.90796400	C	1.33961800	-6.82776400	0.92371000
H	-0.46416500	-7.67026400	1.55196700	H	0.95489100	-7.61301600	1.58174600
H	1.12142800	-7.02356400	1.20520800	H	2.39357300	-6.69926100	1.19755000
C	-0.08458300	-7.36722000	-0.54866200	C	1.22999400	-7.26321300	-0.52778100
H	0.24260000	-8.40181700	-0.68944200	H	1.73309800	-8.22406600	-0.67237400
H	-1.14260700	-7.34952900	-0.83293400	H	0.17972200	-7.43618000	-0.78771800
C	0.70923400	-6.47160600	-1.50980300	C	1.82982600	-6.24781100	-1.51025600
C	0.02277600	-5.09854500	2.57783900	C	1.00280700	-4.98728400	2.58707500

H	1.11532200	-5.05075600	2.62523800	H	2.06964300	-4.74299200	2.60764800
H	-0.31178100	-5.81580500	3.33222300	H	0.82073200	-5.74756600	3.35149300
H	-0.37538300	-4.11650900	2.83776000	H	0.44046000	-4.09118400	2.85374600
C	-1.99534400	-5.51744600	1.16788800	C	-0.94038900	-5.76706500	1.22613800
H	-2.36130400	-4.50275500	1.34352200	H	-1.47585200	-4.82971800	1.39661300
H	-2.39390700	-6.16993200	1.94977700	H	-1.20155900	-6.46661100	2.02510900
H	-2.40291200	-5.85260400	0.21093000	H	-1.30173300	-6.18466000	0.28310000
C	0.22615300	-6.69988700	-2.94476100	C	1.36655600	-6.57156300	-2.93322400
H	0.32551700	-7.75905600	-3.19595500	H	1.65069900	-7.59733200	-3.18194100
H	0.81107400	-6.12387400	-3.66311300	H	1.82263500	-5.90508800	-3.66652800
H	-0.82616000	-6.42645300	-3.06251000	H	0.27992500	-6.49390900	-3.02919200
C	2.21440700	-6.78419900	-1.43417000	C	3.36796800	-6.28359300	-1.46588200
H	2.61801800	-6.66363300	-0.42523000	H	3.76385100	-6.08223000	-0.46683000
H	2.77811300	-6.13161500	-2.10531900	H	3.79077500	-5.54659700	-2.15302400
H	2.38740800	-7.81840400	-1.74301200	H	3.71838900	-7.27264000	-1.77230400
N	1.00380100	-0.52857900	-2.26917400	N	1.03500000	-0.35737600	-2.29442900
C	1.14156900	-1.78947700	-2.65358000	C	1.38941800	-1.57302300	-2.68175000
C	1.60481300	-2.14696600	-3.92936700	C	1.88961200	-1.84508100	-3.96503500
H	1.69666500	-3.19576300	-4.18062600	H	2.16205000	-2.86134100	-4.21937700
C	1.90251000	-1.15272900	-4.82867700	C	1.99575500	-0.81420600	-4.86671900
H	2.24246700	-1.39806000	-5.83009600	H	2.36035100	-0.99655000	-5.87292400
C	1.76190200	0.19331600	-4.44862200	C	1.62800100	0.48683300	-4.48108600
C	2.04835300	1.28754900	-5.32323600	C	1.71043600	1.61829100	-5.35179700
H	2.37205100	1.07089800	-6.33637600	H	2.05479500	1.46577400	-6.36983400
C	1.92064100	2.57197700	-4.90427100	C	1.36912500	2.86017500	-4.92304400
H	2.13894700	3.39493600	-5.57723800	H	1.43582600	3.71108800	-5.59337700
C	1.51034500	2.86622900	-3.56744800	C	0.92955200	3.07450500	-3.58002400
C	1.38383500	4.16990400	-3.06253900	C	0.58731100	4.33380500	-3.06271300
H	1.56162300	5.02024000	-3.71366900	H	0.61075800	5.20687500	-3.70760300
C	1.06002100	4.36995500	-1.74003600	C	0.24655000	4.46603800	-1.73553200
H	0.98845100	5.37380900	-1.34611500	H	0.00779700	5.44007500	-1.33272800
C	0.82670000	3.25355700	-0.92000000	C	0.21565400	3.31978900	-0.92375600
C	1.20551600	1.81094300	-2.68140800	C	0.81997800	1.97766500	-2.69910600
C	1.31588800	0.44804000	-3.13427300	C	1.15973900	0.65690800	-3.16111700
C	0.48643300	3.26846100	0.55066800	C	-0.10978700	3.25648000	0.54884500
N	0.67989600	4.35358400	1.31750400	N	-0.11477600	4.34800200	1.32979100
O	-1.63671400	-0.91819700	-2.19691500	O	-1.48712500	-1.19541300	-2.13691400
N	-2.56241900	-1.50450300	-1.56075300	N	-2.25998100	-1.94931400	-1.47370900
O	-2.50811700	-1.38685600	-0.29807500	O	-2.15650500	-1.85124800	-0.21424000
O	-3.43617600	-2.11843800	-2.11095200	O	-3.04324200	-2.69342000	-1.99939500
N	0.84181200	2.01894800	-1.40720700	N	0.44035900	2.11051700	-1.42066700
O	0.00373600	2.23228800	1.03202200	O	-0.38803700	2.14229000	1.01750800
C	0.21315900	4.29940100	2.71375200	C	-0.54916200	4.19048000	2.72861100
C	1.26093000	3.73867100	3.65767800	C	0.59513400	3.82860500	3.65749400

H -0.69346100 3.69526400 2.73200300	H -1.32407900 3.42464800 2.74577900
H -0.05117500 5.32097600 2.99375700	H -1.00006400 5.14004300 3.02352200
H 0.88252700 3.75025500 4.68265000	H 0.23158200 3.75712500 4.68540400
H 1.50574900 2.70645300 3.39737300	H 1.02868100 2.86445000 3.38258100
H 2.17622800 4.33508900 3.63630700	H 1.38057900 4.58790200 3.63657800
O -2.22005500 1.65368400 -0.89136200	O -2.45075100 1.20161200 -0.89788600
C -5.77819800 1.37505100 -0.87295300	C -5.93126400 0.41370000 -0.90656300
C -6.06267500 0.02295500 -0.71413200	C -6.02340400 -0.96518500 -0.75046100
C -6.79426500 2.32136700 -0.76350700	C -7.07013000 1.20798200 -0.80021100
C -7.36084900 -0.37097800 -0.41584200	C -7.25429900 -1.53814700 -0.45742900
H -5.27931100 -0.71953800 -0.83450700	H -5.14275300 -1.58996100 -0.86797100
C -8.08553600 1.91079900 -0.47007600	C -8.29203900 0.61960100 -0.51188300
H -6.57101200 3.37674700 -0.88986600	H -6.99634800 2.28436300 -0.92492500
H -7.57531100 -1.42873000 -0.29545700	H -7.31858400 -2.61565200 -0.33855600
H -8.87168400 2.65486300 -0.38090900	H -9.17523500 1.24567100 -0.42473500
C -9.80019900 0.12275300 -0.01166500	C -9.74006900 -1.39208300 -0.06101000
H -10.36256600 0.02005200 -0.94556600	H -10.28121400 -1.56754300 -0.99660300
H -10.33334600 0.84824500 0.60665700	H -10.37015100 -0.75117300 0.55958500
H -9.83196200 -0.84398400 0.49424000	H -9.63731400 -2.35627900 0.44022400
C -8.39337900 0.55863400 -0.28956300	C -8.40751300 -0.76267200 -0.33386200
C -4.23753500 2.30162000 -2.56745200	C -4.52222600 1.53000800 -2.60060100
C -4.20535200 1.19410100 -3.60409900	C -4.33096600 0.42401200 -3.62173000
H -3.30591000 2.86627500 -2.56421400	H -3.67637500 2.21641500 -2.59912700
H -5.05686200 2.99573400 -2.76749500	H -5.42734900 2.10313500 -2.81411700
H -4.10449200 1.63198500 -4.60032000	H -4.27457900 0.85967800 -4.62242000
H -3.36253000 0.51988600 -3.44152000	H -3.40977300 -0.13222400 -3.43903500
H -5.12767700 0.60903100 -3.59208500	H -5.16905900 -0.27643800 -3.61320300
C 0.99792400 6.73883200 0.89625100	C -0.26294900 6.75311300 0.92671800
C 1.82586100 7.80846100 0.59172500	C 0.34299800 7.96411900 0.62884400
C 3.70873300 6.33482600 0.46959300	C 2.47367600 6.88075900 0.49213000
C 2.89152600 5.25564000 0.78070300	C 1.88007800 5.66237600 0.79621400
C 1.52976800 5.45425500 0.97986600	C 0.50625400 5.59428500 0.99938400
H -0.06547000 6.89559800 1.05107000	H -1.33608200 6.70129700 1.08499700
H 1.40061600 8.80546000 0.52318100	H -0.26608100 8.86131100 0.56872600
H 4.77063100 6.16892300 0.31354800	H 3.54711600 6.92317700 0.33277300
H 3.30940700 4.25708700 0.86993000	H 2.48228800 4.76206800 0.87633700
C 4.08445600 8.79800400 0.07665300	C 2.36745500 9.37295900 0.11697200
H 5.00946100 8.49079900 -0.41448800	H 3.33662100 9.25261700 -0.37027300
H 4.36148100 9.31373200 1.00188500	H 2.53489800 9.92984500 1.04464400
H 3.58761700 9.53102200 -0.56274600	H 1.74060400 9.99758100 -0.52332100
C 3.19505800 7.62832100 0.37120800	C 1.72062900 8.05202500 0.40454000
$[Am(L3)_2NO_3]^{2+}$-*is3*	**$[Eu(L3)_2NO_3]^{2+}$-*is3***
Am -0.00000100 0.25383900 -0.00001300	Eu -0.00005300 0.25677300 0.00001000

C	-2.82237100	1.68738800	0.86835400	C	-2.79689700	1.68721400	0.87030600
N	-2.30637200	0.59888700	-1.15081200	N	-2.29965000	0.61074900	-1.15251100
C	-3.23201300	1.32405900	-0.53808400	C	-3.22128000	1.33374500	-0.53466600
C	-4.45664700	1.62825200	-1.15421500	C	-4.44437900	1.64828600	-1.15014500
H	-5.22241600	2.17738700	-0.62437400	H	-5.20991900	2.19498100	-0.61733300
C	-4.66381200	1.23009300	-2.45454700	C	-4.65032400	1.26323000	-2.45528300
H	-5.59869200	1.46490700	-2.95397300	H	-5.58394100	1.50558600	-2.95349100
C	-3.66371300	0.52488600	-3.14194800	C	-3.64984000	0.56378300	-3.14869300
C	-3.79170600	0.09970300	-4.50013500	C	-3.76891800	0.15136200	-4.51198900
H	-4.68979700	0.36579200	-5.04831600	H	-4.66348100	0.42191900	-5.06379900
C	-2.81260400	-0.62721800	-5.09475000	C	-2.78589900	-0.57012500	-5.10805000
H	-2.91629600	-0.94962500	-6.12594500	H	-2.88484400	-0.88280100	-6.14272700
C	-1.63390700	-1.00034000	-4.37688900	C	-1.60988300	-0.94985400	-4.38839200
C	-0.62071700	-1.80106100	-4.93167700	C	-0.59177900	-1.74587800	-4.94129400
H	-0.70090100	-2.13562200	-5.96145300	H	-0.66317400	-2.07306100	-5.97409000
C	0.44712800	-2.18008300	-4.15608000	C	0.46962600	-2.13159700	-4.15900700
H	1.22884800	-2.82754400	-4.53137700	H	1.25352700	-2.77793300	-4.53197600
C	0.51585200	-1.72684500	-2.82899000	C	0.52704600	-1.68687900	-2.82866500
N	-0.39088600	-0.91436800	-2.30203700	N	-0.38221900	-0.87717500	-2.30381900
C	-1.46236600	-0.57649900	-3.04126300	C	-1.44748000	-0.53664600	-3.04863100
C	-2.49412600	0.21124900	-2.41831700	C	-2.48401200	0.24168600	-2.42387800
N	1.53225900	-1.84584400	-0.65445800	N	1.50600200	-1.81796400	-0.64015600
C	1.58119500	-2.22172200	-1.93082400	C	1.57654500	-2.18909800	-1.91742100
N	2.48592400	-3.05007200	-2.44027400	N	2.48523400	-3.02108400	-2.41231000
C	3.36899100	-3.58036400	-1.61047100	C	3.34992000	-3.55940300	-1.56810000
C	3.29132600	-3.25519100	-0.23025400	C	3.24984300	-3.23717300	-0.18868200
N	2.39074900	-2.37698800	0.19263700	N	2.34571600	-2.35599800	0.22051100
C	4.17076600	-3.90023600	0.82150100	C	4.10834900	-3.88825600	0.87657000
C	4.44354500	-4.46590600	-2.19862800	C	4.42756400	-4.45176200	-2.13959500
C	5.42188700	-4.48988800	0.15494700	C	5.36665400	-4.48446800	0.22957900
H	6.11574200	-3.67618000	-0.08680500	H	6.06900900	-3.67451600	0.00008800
H	5.94166400	-5.11659100	0.88632800	H	5.87086200	-5.11492900	0.96855400
C	5.11121600	-5.29621600	-1.09421300	C	5.07166800	-5.28752100	-1.02542100
H	6.02952100	-5.73434900	-1.49676700	H	5.99369400	-5.73099500	-1.41330700
H	4.46508100	-6.14439200	-0.84140100	H	4.41609300	-6.13187700	-0.78435300
C	4.59458000	-2.88394100	1.88179200	C	4.52127700	-2.87502800	1.94405300
H	5.12475700	-2.03747800	1.43497100	H	5.06472800	-2.03220400	1.50646400
H	5.27047100	-3.36352400	2.59506500	H	5.18182300	-3.35930100	2.66841200
H	3.73651000	-2.49728000	2.43282500	H	3.65682400	-2.48261700	2.48079400
C	3.34008700	-5.00447800	1.49701700	C	3.26075600	-4.98813100	1.53793100
H	2.45045000	-4.57941000	1.96965800	H	2.36608100	-4.55824300	1.99647000
H	3.93527900	-5.49536600	2.27201900	H	3.84054300	-5.48270100	2.32218200
H	3.00930000	-5.77230900	0.79311300	H	2.93707400	-5.75380800	0.82838500
C	5.46480700	-3.53389900	-2.87616700	C	5.46579600	-3.52624400	-2.80016800

H	6.24522300	-4.13338500	-3.35213100	H	6.24914300	-4.13092200	-3.26456200
H	5.94772400	-2.85510600	-2.16826000	H	5.94257200	-2.85164500	-2.08414900
H	4.98318100	-2.92974400	-3.64894500	H	5.00053000	-2.91804600	-3.57974300
C	3.84789500	-5.39885100	-3.25534000	C	3.84207500	-5.37956000	-3.20657900
H	3.42290400	-4.84207100	-4.09144700	H	3.43401900	-4.81900000	-4.04855400
H	3.06476300	-6.03541100	-2.83347300	H	3.04817600	-6.01123000	-2.79767600
H	4.63262700	-6.05188200	-3.64577900	H	4.62839500	-6.03753900	-3.58530600
N	3.42258100	2.66418800	-1.55297300	N	3.39510400	2.65125600	-1.57306800
C	2.82249000	1.68717300	-0.86842600	C	2.79705200	1.68674700	-0.87035400
N	2.30638700	0.59882100	1.15079500	N	2.29957500	0.61048000	1.15251900
C	3.23207800	1.32390300	0.53804100	C	3.22133000	1.33329100	0.53464800
C	4.45672600	1.62805400	1.15416500	C	4.44445800	1.64770200	1.15013200
H	5.22253400	2.17710600	0.62429200	H	5.21007800	2.19426600	0.61729800
C	4.66384800	1.22996500	2.45452400	C	4.65031900	1.26270000	2.45530000
H	5.59873600	1.46474800	2.95395000	H	5.58396000	1.50495600	2.95351400
C	3.66369400	0.52486100	3.14195400	C	3.64972000	0.56343400	3.14872900
C	3.79164000	0.09976100	4.50017100	C	3.76871000	0.15107000	4.51205100
H	4.68973400	0.36583900	5.04835300	H	4.66330000	0.42153000	5.06386500
C	2.81249000	-0.62707300	5.09481500	C	2.78557800	-0.57025000	5.10812800
H	2.91614600	-0.94941700	6.12603400	H	2.88445900	-0.88288800	6.14282300
C	1.63379000	-1.00018500	4.37695500	C	1.60952300	-0.94985200	4.38846600
C	0.62055200	-1.80082500	4.93177200	C	0.59130100	-1.74571500	4.94138100
H	0.70069700	-2.13532200	5.96157100	H	0.66263000	-2.07286000	5.97419400
C	-0.44729400	-2.17984700	4.15617600	C	-0.47013300	-2.13133600	4.15908600
H	-1.22905200	-2.82724700	4.53150000	H	-1.25412200	-2.77756000	4.53206400
C	-0.51597000	-1.72669400	2.82905500	C	-0.52746800	-1.68667200	2.82872400
C	1.46229700	-0.57642400	3.04129700	C	1.44720300	-0.53668100	3.04868400
C	2.49410100	0.21124200	2.41832600	C	2.48385800	0.24146700	2.42391200
N	-1.53239300	-1.84575900	0.65452600	N	-1.50635900	-1.81777400	0.64018500
C	-1.58132600	-2.22157800	1.93090800	C	-1.57699600	-2.18881700	1.91747200
N	-2.48608000	-3.04987600	2.44040400	N	-2.48580000	-3.02066600	2.41237800
C	-3.36917300	-3.58017600	1.61063700	C	-3.35051700	-3.55893900	1.56817100
C	-3.29150500	-3.25507600	0.23040000	C	-3.25036200	-3.23679300	0.18873800
N	-2.39090700	-2.37692100	-0.19253900	N	-2.34611300	-2.35575400	-0.22047700
C	-4.44376400	-4.46563800	2.19884500	C	-4.42826900	-4.45115800	2.13968000
C	-5.11146100	-5.29599500	1.09448100	C	-5.07243400	-5.28689900	1.02552700
H	-4.46535300	-6.14420900	0.84172500	H	-4.41694300	-6.13133400	0.78451200
H	-6.02978000	-5.73407200	1.49706200	H	-5.99451700	-5.73025700	1.41341100
C	-5.42210400	-4.48973600	-0.15473000	C	-5.36730500	-4.48386900	-0.22951500
H	-6.11594000	-3.67599700	0.08696700	H	-6.06957700	-3.67383000	-0.00007600
H	-5.94189300	-5.11647200	-0.88607500	H	-5.87156500	-5.11430900	-0.96847400
C	-4.17096500	-3.90015800	-0.82131600	C	-4.10892000	-3.88782400	-0.87650400
C	-5.46499400	-3.53353900	2.87631000	C	-5.46641900	-3.52550200	2.80018800
H	-4.98335100	-2.92935700	3.64905700	H	-5.00110800	-2.91732100	3.57975000

H	-6.24544400	-4.13295900	3.35230000	H	-6.24984200	-4.13007800	3.26458800
H	-5.94786900	-2.85476800	2.16835300	H	-5.94310600	-2.85088200	2.08413000
C	-3.84816500	-5.39853300	3.25562800	C	-3.84290200	-5.37897000	3.20671800
H	-3.42315400	-4.84171300	4.09169800	H	-3.43480700	-4.81841700	4.04867800
H	-3.06505900	-6.03515900	2.83381200	H	-3.04906000	-6.01074200	2.79786100
H	-4.63292900	-6.05150000	3.64610800	H	-4.62930000	-6.03685100	3.58545500
C	-3.34031400	-5.00446600	-1.49676100	C	-3.26143600	-4.98782000	-1.53780400
H	-3.93551900	-5.49538900	-2.27173000	H	-3.84126200	-5.48235500	-2.32204800
H	-3.00954600	-5.77225900	-0.79280700	H	-2.93785700	-5.75350600	-0.82822100
H	-2.45066700	-4.57945000	-1.96943000	H	-2.36670300	-4.55805100	-1.99634000
C	-4.59475000	-2.88391800	-1.88166900	C	-4.52171500	-2.87459200	-1.94403600
H	-3.73666800	-2.49730600	-2.43271800	H	-3.65720700	-2.48229500	-2.48077300
H	-5.12491500	-2.03741900	-1.43490300	H	-5.06508400	-2.03169300	-1.50649100
H	-5.27064400	-3.36353000	-2.59492100	H	-5.18229600	-3.35882200	-2.66839100
O	0.60026900	2.59854700	0.88596800	O	0.61151800	2.58732200	0.87686900
N	0.00003600	3.27383700	-0.00009900	N	0.00017200	3.26229000	-0.00008100
O	-0.60010900	2.59842100	-0.88613500	O	-0.61131400	2.58742600	-0.87700100
O	-0.00006300	4.47882500	-0.00012200	O	0.00022600	4.46832000	-0.00004100
N	0.39081900	-0.91429500	2.30206800	N	0.38190900	-0.87709900	2.30386500
O	1.90538100	1.01016800	-1.37712600	O	1.86542300	1.01440400	-1.35854500
C	4.22763000	3.68992400	-0.95767600	C	4.21385600	3.67716200	-0.99708900
C	3.67618600	4.55039400	-0.01441900	C	3.67688600	4.55093500	-0.05762900
C	5.55038600	3.85029100	-1.36290700	C	5.53358900	3.82393700	-1.41656200
C	4.46478700	5.55032500	0.54024000	C	4.47740500	5.55125100	0.47884000
H	2.63647100	4.44587200	0.28088200	H	2.63974300	4.45506800	0.24961100
C	6.32239800	4.85639300	-0.80246000	C	6.31763200	4.83060900	-0.87396100
H	5.97857500	3.17873800	-2.10135200	H	5.95002900	3.14171300	-2.15192700
H	4.02675200	6.21898000	1.27532300	H	4.05102900	6.23047800	1.21108100
H	7.35474900	4.97223300	-1.11936700	H	7.34773100	4.93608100	-1.20163200
C	6.62742800	6.83289600	0.72972800	C	6.65028100	6.82105500	0.63415800
H	6.60323300	7.70869900	0.07295400	H	6.62526300	7.69017500	-0.03140400
H	7.67409100	6.53939600	0.83576800	H	7.69601700	6.52180800	0.73301100
H	6.26233300	7.15076500	1.70806600	H	6.29686700	7.15141000	1.61265000
C	5.79567000	5.72424600	0.15935800	C	5.80577300	5.71209100	0.08345200
C	3.04562200	2.86910600	-2.96464000	C	2.99977400	2.84603000	-2.98111900
C	1.94616200	3.90079400	-3.13551500	C	1.89838900	3.87656300	-3.14669700
H	2.74363200	1.90144100	-3.36345300	H	2.69242500	1.87541700	-3.36873200
H	3.95462700	3.18350900	-3.48207200	H	3.90250500	3.15583100	-3.51211700
H	1.75306500	4.05271800	-4.20034700	H	1.69584900	4.02336600	-4.21051300
H	1.01673000	3.57463000	-2.66507300	H	0.97351500	3.55206400	-2.66646800
H	2.23395100	4.86501600	-2.71047300	H	2.18959900	4.84291000	-2.72892300
O	-1.90531800	1.01032600	1.37708800	O	-1.86536300	1.01473900	1.35850300
C	-4.22735700	3.69026000	0.95749800	C	-4.21307200	3.67809100	0.99700500
C	-3.67591400	4.55062300	0.01414100	C	-3.67583600	4.55165800	0.05750600

C	-5.55008100	3.85072500	1.36278800	C	-5.53273800	3.82532600	1.41652300
C	-4.46449100	5.55055300	-0.54055300	C	-4.47603500	5.55222400	-0.47897200
H	-2.63623300	4.44598700	-0.28124800	H	-2.63873500	4.45542700	-0.24976400
C	-6.32206700	4.85682900	0.80230700	C	-6.31646200	4.83224300	0.87391300
H	-5.97826000	3.17925400	2.10131300	H	-5.94938300	3.14326600	2.15192500
H	-4.02646800	6.21911600	-1.27572600	H	-4.04945500	6.23128400	-1.21124800
H	-7.35439300	4.97275400	1.11926300	H	-7.34651500	4.93807200	1.20161400
C	-6.62706800	6.83323100	-0.73002100	C	-6.64848900	6.82275300	-0.63426200
H	-6.60264200	7.70914600	-0.07340600	H	-6.62307500	7.69192100	0.03122300
H	-7.67378500	6.53984300	-0.83582100	H	-7.69434700	6.52388900	-0.73298000
H	-6.26210800	7.15088300	-1.70848000	H	-6.29505300	7.15289000	-1.61281900
C	-5.79534200	5.72457700	-0.15960700	C	-5.80433900	5.71352000	-0.08354700
C	-1.94578000	3.90112400	3.13527600	C	-1.89736300	3.87687100	3.14636200
H	-2.74345000	1.90187100	3.36339000	H	-2.69205300	1.87601400	3.36864800
H	-3.95431500	3.18407300	3.48188100	H	-3.90169200	3.15684600	3.51204500
H	-1.75272300	4.05315900	4.20010000	H	-1.69466300	4.02369700	4.21014400
H	-1.01635500	3.57480100	2.66493400	H	-0.97265100	3.55201300	2.66606300
H	-2.23344500	4.86532500	2.71010200	H	-2.18828700	4.84328000	2.72853300
C	-3.04533900	2.86952800	2.96448400	C	-2.99911500	2.84669800	2.98098600
N	-3.42232800	2.66452900	1.55283500	N	-3.39463600	2.65193700	1.57298900

Appendix C

Table 1. The LSC data of ^{241}Am(III) and ^{152,154}Eu feed liquids.

Sample	^{241}Am Counts (CPM)	Average	^{152,154}Eu Counts (CPM)	Average
1	7201.67		10955.01	
2	6949.71	6876.61	11289.20	11382.98
3	6478.44		11904.72	

Table 2. The LSC data, distribution ratios and separation factors of ^{241}Am(III) and ^{152,154}Eu in the **L1** acidity experiments.

Acidity (M)	^{241}Am Counts (CPM)	D	^{152,154}Eu Counts (CPM)	D	$SF_{Am(III)/Eu(III)}$
	6413.43	0.07	10736.17	0.06	
0.1	6704.33	0.03	11024.67	0.03	
	6493.25	0.06	10745.12	0.06	
Average		0.05		0.05	1.03
	4937.29	0.39	9710.87	0.17	
0.5	5212.56	0.32	10033.15	0.13	
	4492.56	0.53	9342.15	0.22	
Average		0.41		0.18	2.37
	2505.39	1.74	9094.29	0.25	
1	2992.51	1.30	9782.15	0.16	
	2398.52	1.87	8615.21	0.32	
Average		1.64		0.25	6.67
	732.91	8.38	5734.40	0.99	
2	924.15	6.44	6311.57	0.80	
	653.59	9.52	5476.91	1.08	
Average		8.11		0.96	8.49
	300.34	21.90	3537.55	2.22	
3	462.21	13.88	4725.78	1.41	
	282.12	23.37	3021.12	2.77	
Average		19.72		2.13	9.25
	546.89	11.57	3132.94	2.63	
4	614.63	10.19	3395.19	2.35	
	385.21	16.85	2781.60	3.09	
Average		12.87		2.69	4.78

Table 3. The LSC data, distribution ratios and separation factors of ^{241}Am(III) and ^{152,154}Eu in the **L2** acidity experiments.

Acidity (M)	^{241}Am Counts (CPM)	*D*	^{152,154}Eu Counts (CPM)	*D*	$SF_{Am(III)/Eu(III)}$
	5848.99	0.18	10421.98	0.09	
0.1	5924.12	0.16	10523.15	0.08	
	5792.15	0.19	9991.35	0.14	
Average		0.17		0.10	1.67
	4126.02	0.67	10531.75	0.08	
0.5	4818.29	0.43	10426.93	0.09	
	4303.19	0.60	9925.18	0.15	
Average		0.56		0.11	5.30
	2855.18	1.41	9941.84	0.14	
1	3045.05	1.26	9985.86	0.14	
	2785.59	1.47	9169.57	0.24	
Average		1.38		0.18	7.86
	1646.45	3.18	8965.31	0.27	
2	1844.12	2.73	9392.59	0.21	
	1596.82	3.31	8325.15	0.37	
Average		3.07		0.28	10.85
	1037.69	5.63	8875.57	0.28	
3	1181.25	4.82	9301.83	0.22	
	998.17	5.89	8061.58	0.41	
Average		5.45		0.31	17.79
	1269.47	4.42	8954.87	0.27	
4	1742.62	2.95	9629.92	0.18	
	1063.46	5.47	8741.39	0.30	
Average		4.28		0.25	16.98

Table 4. The LSC data, distribution ratios and separation factors of ^{241}Am(III) and ^{152,154}Eu in the **L3** acidity experiments.

Acidity (M)	^{241}Am Counts (CPM)	*D*	^{152,154}Eu Counts (CPM)	*D*	$SF_{Am(III)/Eu(III)}$
	756.80	8.09	9913.77	0.15	
0.1	1021.18	5.73	10324.52	0.10	
	685.72	9.03	9862.56	0.15	
Average		7.62		0.13	56.43
	239.87	27.67	8158.37	0.40	
0.5	262.41	25.21	8634.15	0.32	
	208.19	32.03	7115.98	0.60	
Average		28.30		0.44	64.65

	186.84	35.80	6385.84	0.78	
1	206.78	32.26	7823.50	0.45	
	149.99	44.85	6295.27	0.81	
Average		37.64		0.68	55.19
	155.12	43.33	5957.72	0.91	
2	176.43	37.98	7792.75	0.46	
	128.72	52.42	5615.29	1.03	
Average		44.58		0.80	55.76
	201.36	33.15	6508.14	0.75	
3	239.61	27.70	8101.24	0.41	
	174.67	38.37	6420.95	0.77	
Average		33.07		0.64	51.49
	178.82	37.46	8161.58	0.39	
4	271.37	24.34	8351.59	0.36	
	291.31	22.61	6625.68	0.72	
Average		28.13		0.49	57.20

Table 5. The LSC data, distribution ratios and separation factors of ^{241}Am(III) and ^{152,154}Eu in the **L3** extractant concentration experiments.

Extractant concentration (mM)	**^{241}Am Counts (CPM)**	***D***	**^{152,154}Eu Counts (CPM)**	***D***
2	4462.59	0.54	11059.30	0.03
4	2310.40	1.98	10598.48	0.07
8	882.49	6.79	9685.92	0.18
12	392.59	16.52	9145.68	0.24
16	269.10	24.55	7985.76	0.43
20	189.92	35.21	6429.58	0.77